

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS	5	Jul 21	Identification of STN records implemented
NEWS	6	Jul 21	Polymer class term count added to REGISTRY
NEWS	7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS	8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS	11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS	12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS	13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS	14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS	17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	18	SEP 22	DIPPR file reloaded
NEWS	19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	EXPRESS		April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS	HOURS		STN Operating Hours Plus Help Desk Availability
NEWS	INTER		General Internet Information
NEWS	LOGIN		Welcome Banner and News Items
NEWS	PHONE		Direct Dial and Telecommunication Network Access to STN
NEWS	WWW		CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 07:07:57 ON 29 SEP 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 07:08:08 ON 29 SEP 2003

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 26 SEP 2003 HIGHEST RN 593958-55-5

DICTIONARY FILE UPDATES: 26 SEP 2003 HIGHEST RN 593958-55-5

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.40

0.61

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:08:14 ON 29 SEP 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

SESSION RESUMED IN FILE 'REGISTRY' AT 07:17:49 ON 29 SEP 2003

FILE 'REGISTRY' ENTERED AT 07:17:49 ON 29 SEP 2003

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.40

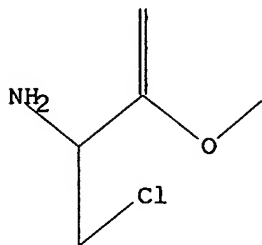
0.61

=>

Uploading 10065677 chloroalananine me ester.str

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 exact full  
FULL SEARCH INITIATED 07:18:14 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.01

L2 4 SEA EXA FUL L1

=> d scan\  
'SCAN\' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN  
SAM - Index Name, MF, and structure - no RN  
FIDE - All substance data, except sequence data  
IDE - FIDE, but only 50 names  
SQIDE - IDE, plus sequence data  
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used  
SQD - Protein sequence data, includes RN  
SQD3 - Same as SQD, but 3-letter amino acid codes are used  
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties  
EPROP - Table of experimental properties  
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract  
APPS -- Application and Priority Information  
BIB -- CA Accession Number, plus Bibliographic Data  
CAN -- CA Accession Number  
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels  
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

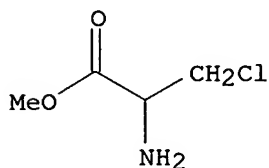
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):end

=> d scan

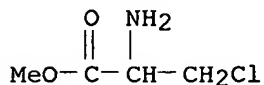
L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN Alanine, 3-chloro-, methyl ester (9CI)  
MF C4 H8 Cl N O2  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

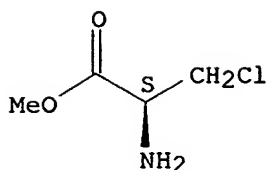
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN L-Alanine, 3-chloro-, methyl ester, labeled with carbon-14 (9CI)  
MF C4 H8 Cl N O2



L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN D-Alanine, 3-chloro-, methyl ester (9CI)  
MF C4 H8 Cl N O2  
CI COM

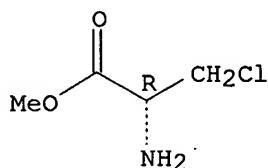
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
 IN L-Alanine, 3-chloro-, methyl ester (9CI)  
 MF C4 H8 Cl N O2  
 CI COM

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
50.55	50.76

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 07:18:57 ON 29 SEP 2003  
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FILE COVERS 1907 - 29 Sep 2003 VOL 139 ISS 14  
 FILE LAST UPDATED: 28 Sep 2003 (20030928/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 12

L3 14 L2

=> d 13 1-14 ti

L3 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Procedure for the production and purification of methyl  
2-(acetamino)-3-chloropropanoate

L3 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI An Aromatization Mechanism of Inactivation of .gamma.-Aminobutyric Acid  
Aminotransferase for the Antibiotic L-Cycloserine

L3 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI A new approach to the synthesis of dipeptides with unnatural amino acids  
using organozinc chemistry

L3 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Synthesis of a phosphinic acid transition state analog inhibitor of  
dihydroorotase

L3 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Synthesis of 6-phosphonoalkyl tetrahydro-4-pyrimidinecarboxylic acids as  
NMDA receptor antagonists

L3 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Preparation of pyridazinones, triazinones, and oxapyridazinones as  
lipoxigenase inhibitors

L3 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Pyridoxal methochloride catalysis of the .beta.-elimination reaction of  
methyl 3-chloroalaninate in water

L3 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Substituted pyridines

L3 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Hydrophilic polymers containing chiral nucleic acid base pendants as  
polynucleotide analogs

L3 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Alteration of GABA metabolism in mammalian brain by L-.alpha.-amino-.beta.-  
chloropropionic acid hydroxamide and related compounds

L3 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI D,L-Cycloserine

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Inhibition of the L-serine O-sulfate-degrading system of pig liver and the  
topography of its active site

L3 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI Inhibition of glutamate dehydrogenase by L-serine O-sulfate and related  
compounds and by photo-oxidation in the presence of Rose Bengal

L3 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI New syntheses of the selenium analogs of dl-cystine and cysteine  
derivatives

=> d 13 14 ti fbib abs

L3 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

TI New syntheses of the selenium analogs of dl-cystine and cysteine derivatives  
 AN 1947:18844 CAPLUS  
 DN 41:18844  
 OREF 41:3758g-i,3759a-b  
 TI New syntheses of the selenium analogs of dl-cystine and cysteine derivatives  
 AU Painter, Edgar Page  
 CS North Dakota Agr. Coll. and Expt. Sta., Fargo  
 SO Journal of the American Chemical Society (1947), 69, 229-32  
 CODEN: JACSAT; ISSN: 0002-7863  
 DT Journal  
 LA Unavailable  
 AB Because of the probable difficulty of sepg. Se compds. from cereals, it seemed that the synthetic route might be the simplest way of showing whether or not the Se amino acids occur in plants. The method of Fredga (C.A. 30, 7101.4) (ClCH<sub>2</sub>CH(NH<sub>2</sub>.HCl)CO<sub>2</sub>Me (I) and K<sub>2</sub>Se<sub>2</sub> in aq. alkali) did not give satisfactory yields, because of the instability of K<sub>2</sub>Se<sub>2</sub> in alkali. I (20 g.) in 150 ml. dioxane, treated with 40 g. K<sub>2</sub>CO<sub>3</sub> and 6 ml. H<sub>2</sub>O and, with cooling, with 32 ml. BzCl, with stirring 4 hrs. at room temp., gives 83% Me .alpha.-benzamido-.beta.-chloropropionate (II), m. 114.degree.. PhSeH (34.3 g.) and 5 g. Na, treated with 17.4 g. I in 75 ml. abs. EtOH, the mixt. refluxed 15 min., 5 ml. concd. HCl added, the unchanged PhSeH oxidized with air, 600 ml. H<sub>2</sub>O and 90 ml. concd. HCl added, the soln. evapd. to near dryness, 400 ml. H<sub>2</sub>O and 1 ml. concd. HCl added, and the soln. shaken with 200 ml. C<sub>6</sub>H<sub>6</sub>, give 56% .beta.-(phenylselenyl)-alanine (III), m. 176-7.degree.; similarly prepd., .beta.-(benzylselenyl)alanine (IV) m. 185.degree., 60% yield; IV was prepd. in 48% yield from II and PhCH<sub>2</sub>SeNa. Reduction of III in NH<sub>3</sub> at -65.degree. with Na gives a nearly quant. yield of Ph<sub>2</sub>Se<sub>2</sub>. However, IV on reduction with Na at the b.p. of liquid NH<sub>3</sub> gives 90% .beta.,.beta.'-diselenodialanine (V), m. 222.degree. (decompn.). I or II with NaHSe in abs. EtOH gives less than 20% V. III is very stable to hydrolysis with concd. HBr but concd. HI slowly cleaved the Ph group.

=> save temp l3 chloroalanines/a  
 CHLOROALANINES/A IS NOT A VALID SAVED NAME  
 Enter the name you wish to use for the saved query,  
 answer set, or L-number list. The name must:  
 1. Begin with a letter,  
 2. Have 1-12 characters,  
 3. Contain only letters (A-Z) and numbers (0-9),  
 4. End with /Q for a query (search profile,  
 structure, or screen set), /A for an answer  
 set, or /L for an L-number list.  
 5. Not already be in use as a saved name,  
 6. Not be END, SAV, SAVE, SAVED  
 7. Not have the form of an L-number (Lnnn).  
 ENTER NAME OR (END):end

=> save temp l3 chloroala/a  
 ANSWER SET L3 HAS BEEN SAVED AS 'CHLOROALA/A'

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	10.43	61.19
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

FILE 'REGISTRY' ENTERED AT 07:24:05 ON 29 SEP 2003  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 26 SEP 2003 HIGHEST RN 593958-55-5  
DICTIONARY FILE UPDATES: 26 SEP 2003 HIGHEST RN 593958-55-5

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STN Note 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e serine methyl ester/cn

E1	1	SERINE LEUKOCYTE PROTEINASE INHIBITOR/CN
E2	1	SERINE METALLOPROTEASE A/CN
E3	1 -->	SERINE METHYL ESTER/CN
E4	1	SERINE METHYL ESTER CYCLIC BUTANEBORONATE/CN
E5	1	SERINE METHYL ESTER HYDROCHLORIDE/CN
E6	1	SERINE MONOSODIUM SALT/CN
E7	1	SERINE MUSTARD/CN
E8	1	SERINE N-(N6-CARBOXY-N2-FORMYL-DL-LYSYL)-, N-BENZYL METHYL E STER, DL-/CN
E9	1	SERINE N-CARBOXY-, N-BENZYL ESTER, IODOACETATE/CN
E10	1	SERINE O-ACETYLTRANSFERASE/CN
E11	1	SERINE O-ACETYLTRANSFERASE (BACILLUS ANTHRACIS STRAIN AMES G ENE CYSE)/CN
E12	1	SERINE O-ACETYLTRANSFERASE (BACILLUS HALODURANS STRAIN C-125 GENE CYSE)/CN

=> e3

L4 1 "SERINE METHYL ESTER"/CN

=> d 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN

RN 2788-84-3 REGISTRY

CN L-Serine, methyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Serine, methyl ester, L- (6CI, 7CI, 8CI)

OTHER NAMES:

CN (S)-Serine methyl ester

CN Methyl L-serinate

CN Methyl serinate

CN **Serine methyl ester**

FS STEREOSEARCH

DR 24425-81-8

MF C4 H9 N O3

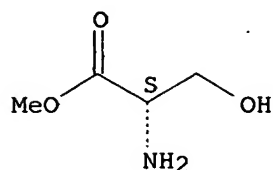
CI COM

LC STN Files: ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,  
CASREACT, CHEMINFORMRX, DDFU, DRUGU, GMELIN\*, IFICDB, IFIPAT, IFIUDB,  
TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)



Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

330 REFERENCES IN FILE CA (1907 TO DATE)  
10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
330 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e thionyl chloride/cn

E1	1	THINK RESIN UPN/CN
E2	1	THINONE RED BROWN BB NEW/CN
E3	0 -->	THINONYL CHLORIDE/CN
E4	1	THINSEC/CN
E5	1	THINSULATE M 400/CN
E6	1	THINTECH/CN
E7	1	THINZ-SPAN/CN
E8	1	THIO 1/CN
E9	1	THIO ALP/CN
E10	1	THIO AMPAC/CN
E11	1	THIO DI-.BETA.-D-GALACTOPYRANOSIDE/CN
E12	1	THIO SOLUBLE BROWN BS/CN

=> e thionyl chloride/cn

E1	1	THIONYL BROMIDE, COMPD. WITH QUINOLINE (1:2)/CN
E2	1	THIONYL BROMIDE, COMPD. WITH QUINOLINE (2:1)/CN
E3	1 -->	THIONYL CHLORIDE/CN
E4	1	THIONYL CHLORIDE (SOCL2)/CN
E5	1	THIONYL CHLORIDE COMPD. WITH METHYL BENZOATE (1:2)/CN
E6	1	THIONYL CHLORIDE COMPOUND WITH DIMETHYLFORMAMIDE (1:2)/CN
E7	1	THIONYL CHLORIDE COMPOUND WITH DIMETHYLFORMAMIDE (1:3)/CN
E8	1	THIONYL CHLORIDE CYANIDE/CN
E9	1	THIONYL CHLORIDE FLUORIDE/CN
E10	1	THIONYL CHLORIDE HYDRIDE/CN
E11	1	THIONYL CHLORIDE NITRATE/CN
E12	5	THIONYL CHLORIDE, ALUMINUM COMPLEX/CN

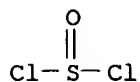
=> e3

L5 1 "THIONYL CHLORIDE"/CN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 7719-09-7 REGISTRY  
CN **Thionyl chloride (8CI, 9CI)** (CA INDEX NAME)  
OTHER NAMES:  
CN Sulfinyl chloride  
CN Sulfinyl dichloride  
CN Sulfur chloride oxide (Cl2SO)  
CN Sulfur chloride oxide (SCl2O)  
CN Sulfur oxychloride  
CN Sulfur oxychloride (SOCl2)

CN Sulfurous dichloride  
 CN Sulfurous oxychloride  
 CN Thionyl chloride (SOCl<sub>2</sub>)  
 CN Thionyl dichloride  
 FS 3D CONCORD  
 MF Cl<sub>2</sub> O S  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD,  
 CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN,  
 CSCHEM, CSNB, DETHERM\*, DIPPR\*, EMBASE, ENCOMPLIT, ENCOMPLIT2,  
 ENCOMPPAT, ENCOMPPAT2, GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA,  
 MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC, PDLCOM\*, PIRA, PROMT, RTECS\*,  
 SPECINFO, SYNTHLINE, TOXCENTER, TULSA, USPAT2, USPATFULL, VTB  
 (\*File contains numerically searchable property data)  
 Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



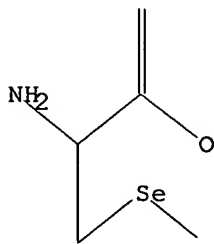
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5337 REFERENCES IN FILE CA (1907 TO DATE)  
 105 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 5344 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 19 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=>  
 Uploading 10065677 selenoalananine.str

L6 STRUCTURE UPLOADED

=> d 16  
 L6 HAS NO ANSWERS  
 L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 16 sss sam  
 SAMPLE SEARCH INITIATED 07:25:47 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 54 TO ITERATE

100.0% PROCESSED 54 ITERATIONS 4 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

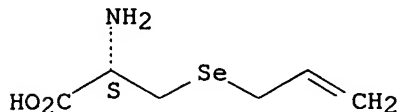
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 640 TO 1520  
PROJECTED ANSWERS: 4 TO 200

L7 4 SEA SSS SAM L6

=> d scan

L7 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN D-Alanine, 3-(2-propenylseleno)- (9CI)  
MF C6 H11 N O2 Se

Absolute stereochemistry.

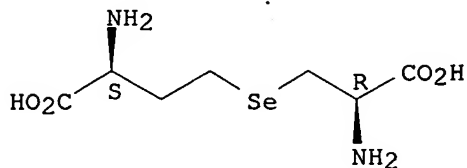


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

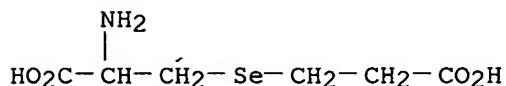
L7 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN Butanoic acid, 2-amino-4-[[ (2R)-2-amino-2-carboxyethyl]seleno]-, (2S)-  
(9CI)  
MF C7 H14 N2 O4 Se

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

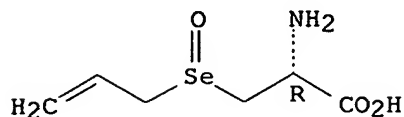
L7 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN Alanine, 3-[(2-carboxyethyl)seleno]- (9CI)  
MF C6 H11 N O4 Se



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN  
IN L-Alanine, 3-(2-propenylseleninyl)- (9CI)  
MF C6 H11 N O3 Se

Absolute stereochemistry.



ALL ANSWERS HAVE BEEN SCANNED

=> search l6 sss full

FULL SEARCH INITIATED 07:26:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1079 TO ITERATE

100.0% PROCESSED 1079 ITERATIONS

102 ANSWERS

SEARCH TIME: 00.00.01

L8 102 SEA SSS FUL L6

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

161.15	222.34
--------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-0.65
------	-------

FILE 'CAPLUS' ENTERED AT 07:26:44 ON 29 SEP 2003

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FILE COVERS 1907 - 29 Sep 2003 VOL 139 ISS 14

FILE LAST UPDATED: 28 Sep 2003 (20030928/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l8

L9 241 L8

=> save temp l9 meseala/a

ANSWER SET L9 HAS BEEN SAVED AS 'MESEALA/A'

=> d his

(FILE 'HOME' ENTERED AT 07:07:57 ON 29 SEP 2003)

FILE 'REGISTRY' ENTERED AT 07:08:08 ON 29 SEP 2003  
L1 STRUCTURE UPLOADED  
L2 4 SEARCH L1 EXACT FULL

FILE 'CAPLUS' ENTERED AT 07:18:57 ON 29 SEP 2003  
L3 14 L2  
SAVE TEMP L3 CHLOROALA/A

FILE 'REGISTRY' ENTERED AT 07:24:05 ON 29 SEP 2003  
E SERINE METHYL ESTER/CN  
L4 1 E3  
E THINONYL CHLORIDE/CN  
E THIONYL CHLORIDE/CN  
L5 1 E3  
L6 STRUCTURE UPLOADED  
L7 4 SEARCH L6 SSS SAM  
L8 102 SEARCH L6 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:26:44 ON 29 SEP 2003  
L9 241 L8  
SAVE TEMP L9 MESEALA/A

=> 14  
L10 330 L4

=> 15  
L11 5350 L5

=> 110(1)111  
L12 0 L10(L)L11

=> 110 and 19  
L13 1 L10 AND L9

=> d 113 ti fbib abs

L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Synthesis of [3,14-L-selenocysteine, 8-D-tryptophan]somatostatin  
AN 1981:157223 CAPLUS  
DN 94:157223  
TI Synthesis of [3,14-L-selenocysteine, 8-D-tryptophan]somatostatin  
AU Hartrodt, B.; Neubert, K.; Bierwolf, B.; Blech, W.; Jakubke, H. D.  
CS Physiol-Chem. Inst., Martin-Luther Univ., Halle/Salle, 402, Ger. Dem. Rep.  
SO Tetrahedron Letters (1980), 21(25), 2393-6  
CODEN: TELEAY; ISSN: 0040-4039  
DT Journal  
LA German  
AB The title compd. (I) was prepd. by conventional peptide condensation reactions. in soln. The inhibitory power of I for insulin and glucagon secretion in rats was similar to that of the natural peptide hormone.

=> save temp all selenocmpds/1  
L# LIST L1-L13 HAS BEEN SAVED AS 'SELENOCMPDS/L'

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.08	226.42
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-1.30

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 07:29:14 ON 29 SEP 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS	5	Jul 21	Identification of STN records implemented
NEWS	6	Jul 21	Polymer class term count added to REGISTRY
NEWS	7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS	8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS	11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS	12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS	13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS	14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS	17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	18	SEP 22	DIPPR file reloaded
NEWS	19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	20	SEP 29	DISSABS now available on STN
NEWS EXPRESS			OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information

NEWS LOGIN      Welcome Banner and News Items  
NEWS PHONE      Direct Dial and Telecommunication Network Access to STN  
NEWS WWW        CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 11:56:41 ON 08 OCT 2003

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'STNGUIDE' ENTERED AT 11:56:53 ON 08 OCT 2003  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Oct 3, 2003 (20031003/UP).

=> FIL HOME

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	0.27

FILE 'HOME' ENTERED AT 11:57:00 ON 08 OCT 2003

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.48

FILE 'STNGUIDE' ENTERED AT 11:57:05 ON 08 OCT 2003  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Oct 3, 2003 (20031003/UP).

=> DIS SAVED

NAME	CREATED	NOTES/TITLE
ACRYLMETATH/A	TEMP	67 ANSWERS IN FILE CAPLUS
ALKYLATIN/L	13 DEC 2001	9 L-NUMBERS
CHLOROALA/A	TEMP	14 ANSWERS IN FILE CAPLUS
ESTERODOR/L	05 SEP 2002	42 L-NUMBERS
HYDROXAMINES/A	TEMP	8641 ANSWERS IN FILE CAPLUS
INDIUMCL3/A	30 MAY 2001	1 ANSWER IN FILE REGISTRY
LTWENTAUGFOR/A	04 AUG 2001	72 ANSWERS IN FILE CAPLUS
MESEALA/A	TEMP	241 ANSWERS IN FILE CAPLUS
METATHESIS/L	TEMP	36 L-NUMBERS
METHIDES/A	TEMP	500 ANSWERS IN FILE CAPLUS

NEOTAMECRYST/A	24 APR 2001	59 ANSWERS IN FILE CAPLUS
NVLARMFULGEN/A	19 APR 2001	196 ANSWERS IN FILE REGISTRY
POHBENZALDEH/A	10 JUL 2001	5519 ANSWERS IN FILE CAPLUS
POLYINHBT/L	TEMP	15 L-NUMBERS
PROSTACMPD15/A	01 AUG 2001	34 ANSWERS IN FILE CAPLUS
SELENOCMPDS/L	TEMP	13 L-NUMBERS
STILLEAPP/L	07 JAN 2002	17 L-NUMBERS
TWOAMINOPOLY/Q	16 APR 2001	UPLOADED STRUCTURE

=> DIS SAVED/S  
NO SAVED SDI REQUESTS

=> FIL CAPLUS		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.06	0.54

FILE 'CAPLUS' ENTERED AT 11:57:35 ON 08 OCT 2003  
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FILE COVERS .1907 - 8 Oct 2003 VOL 139 ISS 15  
FILE LAST UPDATED: 7 Oct 2003 (20031007/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> ACT CHLOROALA/A  
L1 STR  
L2 ( 4)SEA FILE=REGISTRY EXA FUL L1  
L3 14 SEA FILE=CAPLUS ABB=ON PLU=ON L2

=> ACT MESEALA/A  
L4 STR  
L5 ( 102)SEA FILE=REGISTRY SSS FUL L4  
L6 241 SEA FILE=CAPLUS ABB=ON PLU=ON L5

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	0.96

FILE 'REGISTRY' ENTERED AT 11:58:15 ON 08 OCT 2003  
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Property values tagged with IC are from the ZIC/VINITI data file



provided by InfoChem.

STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2  
DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e dimethyldiselenide/cn

E1	1	DIMETHYLDIPROPYLTIN COMPOUND WITH IODINE (1:1)/CN
E2	1	DIMETHYLDIPYRROLIDINOSILANE/CN
E3	0 -->	DIMETHYLDISELENIDE/CN
E4	1	DIMETHYLDISILANE-ETHYLENE OXIDE ADDUCT/CN
E5	1	DIMETHYLDISILAZANE/CN
E6	1	DIMETHYLDISOYA ALKYL, CHLORIDES QUATERNARY AMMONIUM COMPOUND S/CN
E7	1	DIMETHYLDISOYA ALKYLAMMONIUM CHLORIDES/CN
E8	1	DIMETHYLDISTAMYCIN A/CN
E9	1	DIMETHYLDISTEARYL AMMONIUM 5-SULFOISOPHTHALATE-PROPYLENE GLY COL-DIETHYLENE GLYCOL-DIMETHYL TEREPHTHALATE COPOLYMER STEAR ATE/CN
E10	1	DIMETHYLDISTEARYLAMMONIUM/CN
E11	1	DIMETHYLDISTEARYLAMMONIUM ACETATE/CN
E12	1	DIMETHYLDISTEARYLAMMONIUM BOROHYDRIDE/CN

=> e dimethyl diselenide/cn

E1	1	DIMETHYL DIPROPARGYLMALONATE/CN
E2	1	DIMETHYL DIPROPYLMALONATE/CN
E3	1 -->	DIMETHYL DISELENIDE/CN
E4	1	DIMETHYL DISELENIDE RADICAL CATION/CN
E5	1	DIMETHYL DISELENIDE(1+)/CN
E6	1	DIMETHYL DISULFIDE/CN
E7	1	DIMETHYL DISULFIDE CATION RADICAL/CN
E8	1	DIMETHYL DISULFIDE RADICAL ANION(1-)/CN
E9	1	DIMETHYL DISULFIDE RADICAL CATION/CN
E10	1	DIMETHYL DISULFIDE RADICAL CATION(1+)/CN
E11	1	DIMETHYL DISULFIDE TETRAOXIDE/CN
E12	1	DIMETHYL DISULFIDE(1+)/CN

=> \e3

L7	2128 \E3
	(E3)

=> \e3

L8	2128 \E3
	(E3)

=> e3

L9	1 "DIMETHYL DISELENIDE"/CN
----	----------------------------

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 7101-31-7 REGISTRY

CN Diselenide, dimethyl (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Methyl diselenide (6CI, 7CI, 8CI)  
 OTHER NAMES:  
 CN **Dimethyl diselenide**  
 MF C2 H6 Se2  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA,  
 CANCERLIT, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX,  
 CHEMLIST, CSCHEM, DDFU, DETHERM\*, DRUGU, GMELIN\*, MEDLINE, NIOSHTIC,  
 PROMT, TOXCENTER, USPATFULL, VETU  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

H<sub>3</sub>C-Se-Se-CH<sub>3</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

354 REFERENCES IN FILE CA (1907 TO DATE)  
 356 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e methyl selenol

E1	12844467	METHYL/BI
E2	1	METHYL CARBAMATO-N/BI
E3	0 -->	METHYL SELENOL/BI
E4	1	METHYL'/BI
E5	3	METHYL, 1, 2, 3, 4/BI
E6	1	METHYL, 2, 2A:METHYL', 3B, 3C/BI
E7	1	METHYL, 4/BI
E8	1	METHYL, 6'/BI
E9	3	METHYL, METHYL, 3, 4/BI
E10	1	METHYL, METHYL, METHYL/BI
E11	1	METHYL, METHYL, METHYL, 2, 4, 4/BI
E12	5	METHYL, METHYL, METHYL, 3, 3, 4, 4/BI

=> e methyl selenol/cn

E1	1	METHYL SELENIUM PHOSPHORODITHIOATE ((MEO)2PS2)2SE)/CN
E2	1	METHYL SELENOBENZOATE/CN
E3	0 -->	METHYL SELENOL/CN
E4	1	METHYL SELENONE/CN
E5	1	METHYL SELENOXIDE/CN
E6	1	METHYL SELENOXIDE, COMPD. WITH CADMIUM CHLORIDE (2:1)/CN
E7	1	METHYL SELENOXIDE, COMPD. WITH COBALT CHLORIDE (COCL2) (2:1)/CN
E8	1	METHYL SELENOXIDE, COMPD. WITH COPPER CHLORIDE (CUCL2) (2:1)/CN
E9	1	METHYL SELENOXIDE, COMPD. WITH MERCURY CHLORIDE (HGCL2) (1:1)/CN
E10	1	METHYL SELENOXIDE, COMPD. WITH NICKEL BROMIDE (NIBR2) (3:2)/CN
E11	1	METHYL SELENOXIDE, COMPD. WITH NICKEL CHLORIDE (NICL2) (3:2)/CN
E12	1	METHYL SELENOXIDE, COMPD. WITH NITROGEN OXIDE (N2O4) (1:1)/CN

=> e methyl selenide/cn

E1	1	METHYL SELENATE ((MEO)2SE2O5)/CN
----	---	----------------------------------

E2 1 METHYL SELENATE ((MEO)2SEO2)/CN  
 E3 1 --> METHYL SELENIDE/CN  
 E4 1 METHYL SELENIDE, BROMINE COMPLEX/CN  
 E5 1 METHYL SELENIDE, COMPD. WITH BBR3/CN  
 E6 1 METHYL SELENIDE, COMPD. WITH BF3/CN  
 E7 1 METHYL SELENIDE, COMPD. WITH BH3/CN  
 E8 1 METHYL SELENIDE, COMPD. WITH BORON BROMIDE (BBR3) (1:1)/CN  
 E9 1 METHYL SELENIDE, COMPD. WITH BORON CHLORIDE (BCL3) (1:1)/CN  
 E10 1 METHYL SELENIDE, COMPD. WITH BORON FLUORIDE (BF3) (1:1)/CN  
 E11 1 METHYL SELENIDE, COMPD. WITH BORON IODIDE (BI3) (1:1)/CN  
 E12 1 METHYL SELENIDE, COMPD. WITH IODINE (1:1)/CN

=> e3

L10 1 "METHYL SELENIDE"/CN

=> d 110

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 593-79-3 REGISTRY  
 CN Methane, selenobis- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Methyl selenide (6CI, 7CI, 8CI)  
 OTHER NAMES:  
 CN Dimethyl selenide  
 CN Dimethylselenium  
 CN Methyl selenium  
 MF C2 H6 Se  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
 BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS,  
 CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM\*, EMBASE, GMELIN\*, HODOC\*,  
 MEDLINE, MSDS-OHS, NIOSHTIC, PIRA, PROMT, RTECS\*, SPECINFO, TOXCENTER,  
 USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)

H<sub>3</sub>C-Se-CH<sub>3</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

614 REFERENCES IN FILE CA (1907 TO DATE)  
 7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 615 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.84	22.80

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FILE COVERS 1907 - 8 Oct 2003 VOL 139 ISS 15  
FILE LAST UPDATED: 7 Oct 2003 (20031007/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 19

L11 356 L9

=> d his

(FILE 'HOME' ENTERED AT 11:56:41 ON 08 OCT 2003)

FILE 'STNGUIDE' ENTERED AT 11:56:53 ON 08 OCT 2003

FILE 'HOME' ENTERED AT 11:57:00 ON 08 OCT 2003

FILE 'STNGUIDE' ENTERED AT 11:57:05 ON 08 OCT 2003

FILE 'CAPLUS' ENTERED AT 11:57:35 ON 08 OCT 2003

ACT CHLOROALA/A

-----

L1 STR

L2 ( 4)SEA FILE=REGISTRY EXA FUL L1

L3 14 SEA FILE=CAPLUS ABB=ON PLU=ON L2

-----

ACT MESEALA/A

-----

L4 STR

L5 ( 102)SEA FILE=REGISTRY SSS FUL L4

L6 241 SEA FILE=CAPLUS ABB=ON PLU=ON L5

-----

FILE 'REGISTRY' ENTERED AT 11:58:15 ON 08 OCT 2003

E DIMETHYLDISELENIDE/CN

E DIMETHYL DISELENIDE/CN

L7 2128 \E3

L8 2128 \E3

L9 1 E3

E METHYL SELENOL

E METHYL SELENOL/CN

E METHYL SELENIDE/CN

L10 1 E3

FILE 'CAPLUS' ENTERED AT 12:00:49 ON 08 OCT 2003

L11 356 L9

=> l11 and 16

L12 8 L11 AND L6

=> d l12 1-8 ti

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN

TI Soil methylation-demethylation pathways for metabolism of plant-derived

selenoamino acids

- L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Methylation of inorganic and organic selenium by the bacterial thiopurine methyltransferase
- L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical
- L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Dimethyldiselenide and methylseleninic acid generate superoxide in an in vitro chemiluminescence assay in the presence of glutathione: Implications for the anticarcinogenic activity of L-selenomethionine and L-Se-methylselenocysteine
- L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Thioredoxin reductase activity in rat liver is not affected by supranutritional levels of monomethylated selenium in vivo and is inhibited only by high levels of selenium in vitro
- L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Allium chemistry: synthesis, natural occurrence, biological activity, and chemistry of Se-alk(en)ylselenocysteines and their .gamma.-glutamyl derivatives and oxidation products
- L12 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Biotransformations of Selenium Oxyanion by Filamentous Cyanophyte-Dominated Mat Cultured from Agricultural Drainage Waters
- L12 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Selenium-77 relaxation time studies on compounds of biological importance: dialkyl selenides, dialkyl diselenides, selenols, selenonium compounds, and seleno oxyacids

=> d l12 3 ti fbib abs

- L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical  
 AN 2002:364013 CAPLUS  
 DN 136:369993  
 TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical  
 IN Spallholz, Julian E.; Reid, Ted W.; Walkup, Robert D.  
 PA Pharmase, Incorporated, USA  
 SO Eur. Pat. Appl., 21 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1
- | PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| EP 1205471  | A1   | 20020515 | EP 2001-103018  | 20010208 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR |      |          |                 |          |
| US 2000-677563 A 20001002   |      |          |                 |          |
| EP 1077209  | A1   | 20010221 | EP 2000-117106  | 20000809 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO                 |      |          |                 |          |
| US 1999-376073 A 19990816   |      |          |                 |          |
| US 2003083383   | A1   | 20030501 | US 2002-288024  | 20021105 |
| US 1999-376073 B219990816   |      |          |                 |          |
| US 2000-677563 A320001002   |      |          |                 |          |
- OS CASREACT 136:369993

AB The invention describes the synthesis and use of L-Se-methylselenocysteine (I), a nutraceutical which is less toxic than L-selenomethionine towards normal cells. The synthesis involves mixing N-(tert-butoxycarbonyl)-L-serine with a dialkyl diazodicarboxylate and at least one of a trialkylphosphine, triarylphosphine and phosphite to form a mixt. contg. N-(tert-butoxycarbonyl)-L-serine .beta.-lactone, addn. of methylselenol or a salt, and deprotection. This synthesis significantly improves the manufg. efficiency and utility I., a naturally occurring rare form of org. selenium. I formed in this manner may be used as a nutraceutical in the diets of humans or animals for various beneficial purposes, such as, for example, to prevent or reduce the risk of developing cancer. A bar graph which compares the effect of I and L-selenomethionine on the growth of normal rabbit fibroblasts is given.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	8.60	31.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2  
DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e L-Se-methylselenocysteine/cn

E1	1	L-SDDCTP/CN
E2	1	L-SE/CN
E3	0 -->	L-SE-METHYLSELENOCYSTEINE/CN
E4	1	L-SEC-AMYL ALCOHOL/CN
E5	1	L-SECURININE/CN
E6	1	L-SELECTIN (BABOON PRECURSOR)/CN.
E7	1	L-SELECTIN (CATTLE PRECURSOR REDUCED)/CN
E8	1	L-SELECTIN (HUMAN CLONE 9628221 GENE SELL REFERENCE ISOFORM)/CN
E9	1	L-SELECTIN (HUMAN CLONE B125 LEUKOCYTE ADHESION MOLECULE PRECURSOR REDUCED)/CN
E10	1	L-SELECTIN (HUMAN GENE SELL ISOFORM 1)/CN
E11	1	L-SELECTIN (HUMAN GENE SELL ISOFORM 10)/CN

E12 1 L-SELECTIN (HUMAN GENE SELL ISOFORM 11)/CN

=> e methylselenocysteine/cn

E1 1 METHYLSELENOCYANATE/CN  
E2 1 METHYLSELENOCYANIDE/CN  
E3 2 --> METHYLSELENOCYSTEINE/CN  
E4 1 METHYLSELENOL/CN  
E5 1 METHYLSELENOMAGNESIUM BROMIDE/CN  
E6 1 METHYLSELENOMAGNESIUM IODIDE/CN  
E7 1 METHYLSELENOMETHIONINE/CN  
E8 1 METHYLSELENOMETHYLLITHIUM/CN  
E9 1 METHYLSELENYL CHLORIDE/CN  
E10 1 METHYLSELENOCHOLINE/CN  
E11 1 METHYLSEMIQUARIC ACID ION(1-)/CN  
E12 1 METHYLSILAIISONITRILE/CN

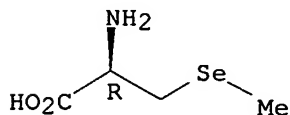
=> e3

L13 2 METHYLSELENOCYSTEINE/CN

=> d l13 1-2

L13 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 26046-90-2 REGISTRY  
CN L-Alanine, 3-(methylseleno)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, 3-(methylselenyl)-, L- (8CI)  
OTHER NAMES:  
CN 3-(Methylseleno)-L-alanine  
CN Methylseleno-L-cysteine  
CN **Methylselenocysteine**  
CN Se-Methylselenocysteine  
FS STEREOSEARCH  
MF C4 H9 N O2 Se  
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT,  
CHEMCATS, CSCHEM, DDFU, DRUGU, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)

Absolute stereochemistry.

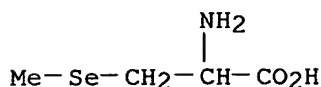


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

80 REFERENCES IN FILE CA (1907 TO DATE)  
80 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L13 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 2574-71-2 REGISTRY  
CN Alanine, 3-(methylseleno)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, 3-(methylselenyl)- (6CI, 7CI, 8CI)  
OTHER NAMES:  
CN DL-Se-methylselenocysteine  
CN **Methylselenocysteine**  
CN NSC 319053  
CN Selenocysteine, Se-methyl-  
DR 26145-42-6  
MF C4 H9 N O2 Se

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CANCERLIT, CAOLD,  
CAPLUS, CHEMCATS, MEDLINE, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

34 REFERENCES IN FILE CA (1907 TO DATE)  
34 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	8.38	39.78
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.65

FILE 'CAPLUS' ENTERED AT 12:07:01 ON 08 OCT 2003  
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FILE COVERS 1907 - 8 Oct 2003 VOL 139 ISS 15  
FILE LAST UPDATED: 7 Oct 2003 (20031007/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 113  
L14 112 L13  
  
=> 113/prep  
112 L13  
3060787 PREP/RL  
L15 10 L13/PREP  
(L13 (L) PREP/RL)  
  
=> d 115 1-10 ti

L15 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Soil methylation-demethylation pathways for metabolism of plant-derived



selenoamino acids

- L15 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical
- L15 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Chemoprevention of mammary cancer with Se-Allylselenocysteine and other selenoamino acids in the rat
- L15 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Synthesis and structure characterization of selenium metabolites
- L15 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Synthesis of Novel Se-Substituted Selenocysteine Derivatives as Potential Kidney Selective Prodrugs of Biologically Active Selenol Compounds: Evaluation of Kinetics of .beta.-Elimination Reactions in Rat Renal Cytosol
- L15 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Chemical form of selenium, critical metabolites, and cancer prevention
- L15 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Preparation of sulfur and selenium amino acids with microbial pyridoxal phosphate enzymes
- L15 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Selenium-containing amino acids
- L15 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Enzymatic synthesis of selenium-substituted L-selenocysteine with tryptophan synthase
- L15 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Selenoamino acids

=> d 115 1-10 ti fbib abs

- L15 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Soil methylation-demethylation pathways for metabolism of plant-derived selenoamino acids  
AN 2002:947285 CAPLUS  
DN 138:136504  
TI Soil methylation-demethylation pathways for metabolism of plant-derived selenoamino acids  
AU Martens, Dean A.; Suarez, Donald L.  
CS Southwest Watershed Research Center, Agricultural Research Service, U.S. Department of Agriculture, Tucson, AZ, 85719, USA  
SO ACS Symposium Series (2003), 835(Biogeochemistry of Environmentally Important Trace Elements), 355-369  
CODEN: ACSMC8; ISSN: 0097-6156  
PB American Chemical Society  
DT Journal  
LA English  
AB There is conflicting field information about Se toxicity in waterfowl and fish, based on criteria of total Se concn. At least part of this uncertainty is due to the difference in toxicity assocd. with various Se species. There is toxicity data on the selenoamino acid selenomethionine (SeMet) to avian species, but little is known on the environmental transformations of SeMet and the possible intermediates of org. Se decompn. To det. the potential decompn. of Se amino acids, methylation and demethylation pathway intermediates for the transformations of sulfur (S) amino acids, identified from aerobic marine sediments, were compared

to potential analog Se intermediates synthesized for this study. Two terrestrial soils with apparently different pathways for metabolizing SeMet were treated with 25 .mu.g S intermediate-S g-1 soil and the soil headspace analyzed for the methylation pathway gas dimethylsulfide (DMS) or the demethylation pathway gas dimethyldisulfide (DMDS). Addn. of S-methylmethionine (MMet), and dimethylsulfoniopropionic acid (DMSP) to the Panhill and Panoche soils resulted in only DMS evolution; addn. of 3-(methylthio)propionic acid (MTP) resulted in DMDS in the soils and 3-mercaptopropionic acid (MCP) addn. was not volatilized confirming that terrestrial soil S pathways are similar to documented marine pathways. The Panhill soil evolved only DMDS as a result of the methionine (Met) demethylation pathway and the Panoche soil evolved only DMS from the methylation of Met. The evolution of Se gases dimethylselenide (DMSe) and dimethyldiselenide (DMDSe) from addn. of SeMet, methylselenomethionine (MSeMet), and dimethylselenopropionic acid (DMSeP) followed the same pattern as noted with the S products. DMSe evolved from a methylation pathway and DMDSe evolved from a demethylation metab. Selenocystine (SeCys) and a methylated selenocysteine (MSeCys) added to the two soils showed limited volatilization as DMSe. A large portion of the Se not volatilized from soil was found as a non-amino acid org. selenide compd.(s) and these unidentified intermediate compds. may be present in significant concns. in some environments. The different metabolic pathways of Se in soils may explain why in certain waterfowl areas Se-induced problems have not been found where predicted based on total Se concns.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical  
AN 2002:364013 CAPLUS  
DN 136:369993  
TI A method of using synthetic L-Se-methylselenocysteine as a nutraceutical  
IN Spallholz, Julian E.; Reid, Ted W.; Walkup, Robert D.  
PA Pharmase, Incorporated, USA  
SO Eur. Pat. Appl., 21 pp.  
CODEN: EPXXDW

DT Patent  
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1205471	A1	20020515	EP 2001-103018	20010208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EP 1077209	A1	20010221	EP 2000-117106	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2003083383	A1	20030501	US 1999-376073 A	19990816
			US 2002-288024	20021105
			US 1999-376073 B2	19990816
			US 2000-677563 A3	20001002

OS CASREACT 136:369993

AB The invention describes the synthesis and use of L-Se-methylselenocysteine (I), a nutraceutical which is less toxic than L-selenomethionine towards normal cells. The synthesis involves mixing N-(tert-butoxycarbonyl)-L-serine with a dialkyl diazodicarboxylate and at least one of a trialkylphosphine, triarylphosphine and phosphite to form a mixt. contg. N-(tert-butoxycarbonyl)-L-serine .beta.-lactone, addn. of methylselenol or a salt, and deprotection. This synthesis significantly improves the manufg. efficiency and utility I., a naturally occurring rare form of org. selenium. I formed in this manner may be used as a nutraceutical in the

diets of humans or animals for various beneficial purposes, such as, for example, to prevent or reduce the risk of developing cancer. A bar graph which compares the effect of I and L-selenomethionine on the growth of normal rabbit fibroblasts is given.

RE.CNT 8        THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Chemoprevention of mammary cancer with Se-Allylselenocysteine and other selenoamino acids in the rat  
AN 2000:69937 CAPLUS  
DN 132:307715  
TI Chemoprevention of mammary cancer with Se-Allylselenocysteine and other selenoamino acids in the rat  
AU Ip, Clement; Zhu, Zongjian; Thompson, Henry J.; Lisk, Donald; Ganther, Howard E.  
CS Department of Experimental Pathology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA  
SO Anticancer Research (1999), 19(4B), 2875-2880  
CODEN: ANTRD4; ISSN: 0250-7005  
PB International Institute of Anticancer Research  
DT Journal  
LA English  
AB The present study examd. the mammary cancer chemopreventive activity of Se-methylselenocysteine, Se-propylselenocysteine and Se-allylselenocysteine in the rat methylnitrosourea (MNU) model. Each compd. was supplemented in the diet at a level of 2 ppm Se for the entire duration of the expt. after MNU dosing. Se-allylselenocysteine was the most active and caused a redn. in total tumor yield by 86%. Se-methylselenocysteine and Se-propylselenocysteine were similar but less effective, and both produced a decrease of about 50% in tumorigenesis. All 3 compds. were very well absorbed through the gastrointestinal tract. However, more Se was excreted in urine after gavaging with Se-propylselenocysteine or Se-allylselenocysteine compared with Se-methylselenocysteine. Anal. of Se in the mammary gland and other organs showed that tissue Se levels did not appear to be correlated with differences in chemopreventive activity. A lyase activity capable of catalyzing scission of the Se-alkyl group from the remainder of the amino acid was demonstrated. This activity was high in liver and kidney, but relatively low in mammary gland and intestine. Minimal variations in enzyme activity towards each of the substrates were obsd. These results support the concept that Se-alkylselenoamino acids could be used as precursors for delivering the Se-alkyl moiety and that intrinsic chem. differences in the Se-alkyl substituent of the test compds. are likely to be important determinants of their biol. effects.

RE.CNT 44       THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD  
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Synthesis and structure characterization of selenium metabolites  
AN 1998:278784 CAPLUS  
DN 129:64137  
TI Synthesis and structure characterization of selenium metabolites  
AU Fan, Teresa W. -M.; Lane, Andrew N.; Martens, Dean; Higashi, Richard M.  
CS Department of Land, Air and Water Resources, University of California, Davis, CA, 95616-8627, USA  
SO Analyst (Cambridge, United Kingdom) (1998), 123(5), 875-884  
CODEN: ANALAO; ISSN: 0003-2654  
PB Royal Society of Chemistry  
DT Journal  
LA English  
AB The difficulty in detg. trace-level organoseleno metabolites and the lack of com. available stds. have been major barriers to a mol.-level

understanding of Se biogeochem., ecotoxicol. and nutrition, particularly in aquatic ecosystems. To overcome the problem, three important precursors of volatile alkyl selenides were synthesized, including dimethylselenonium propionate (DMSeP), which has only been postulated to exist in nature. A combination of 2-D multinuclear NMR, electro-spray MS and GC-MS methods was employed to identify DMSeP, methylselenomethionine and methylselenocysteine in synthetic preps. without extensive clean-up. An alk. hydroelimination test coupled with GC-MS anal. for the release pattern of di-Me selenide (DMSe) and di-Me diselenide (DMDS<sub>2</sub>) was developed for a diagnostic detn. of the three products. The DMSe release pattern of DMSeP confirmed the presence of a DMSeP-like compd. in the biomass of 100 mg l-l Se-treated *Chlorella* investigated previously. Silylation-GC-MS was tested for the detn. of selenomethionine, selenocysteine and methylselenocysteine in a std. mixt. with a detection limit of better than 1 pmol per 0.5 .mu.l injection vol. for selenomethionine. This method was applied to the anal. of the acid digest of the proteinaceous fraction of the *Chlorella* culture. Selenomethionine was found to contain >70% of the protein-bound Se, although this constituted only a minor fraction of the total Se in the *Chlorella* biomass. These findings revealed the metabolic relationship between Se volatilization and selenomethionine incorporation into proteins. This knowledge is crit. to advancement in Se biogeochem., ecotoxicol. and the development of in situ bioremediation schemes.

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Synthesis of Novel Se-Substituted Selenocysteine Derivatives as Potential Kidney Selective Prodrugs of Biologically Active Selenol Compounds: Evaluation of Kinetics of .beta.-Elimination Reactions in Rat Renal Cytosol

AN 1996:241974 CAPLUS

DN 124:306525

TI Synthesis of Novel Se-Substituted Selenocysteine Derivatives as Potential Kidney Selective Prodrugs of Biologically Active Selenol Compounds: Evaluation of Kinetics of .beta.-Elimination Reactions in Rat Renal Cytosol

AU Andreadou, Ioanna; Menge, Wiro M. P. B.; Commandeur, Jan N. M.; Worthington, Eduard A.; Vermeulen, Nico P. E.

CS Leiden Amsterdam Center for Drug Research, Vrije Universiteit Amsterdam, Amsterdam, 1081 HV, Neth.

SO Journal of Medicinal Chemistry (1996), 39(10), 2040-6  
CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB Eighteen Se-substituted selenocysteine derivs. were prepd. as potential kidney selective prodrugs which can be activated by renal cysteine conjugate .beta.-lyase to selenium-contg. chemoprotectants or antitumor agents. Selenocysteine derivs. with aliph. and benzylic Se-substituents were synthesized by reducing selenocystine to selenocysteine followed by a reaction with the corresponding alkyl and benzyl halogenides. Selenocysteine derivs. with arom. Se-substituents were synthesized by reaction of .beta.-chloroalanine with substituted phenylselenol compds., which were formed by reducing substituted di-Ph diselenides by NaBH<sub>4</sub>. The enzyme kinetic parameters (apparent K<sub>m</sub> and V<sub>max</sub>) of the .beta.-elimination reaction of the selenocysteine conjugates were studied in rat renal cytosol. The results suggest that Se-substituted L-selenocysteine conjugates are extremely good substrates for renal cysteine conjugate .beta.-lyases as indicated by low apparent K<sub>m</sub> and high V<sub>max</sub> values. The benzyl-substituted Se-conjugates appeared to be better substrates than the phenyl- and alkyl-substituted Se-conjugates. Corresponding L-cysteine S-conjugates were too poor substrates to obtain proper enzyme kinetics.

Recently, local activation of cysteine S-conjugates by renal cysteine conjugate .beta.-lyases was proposed as a new strategy to target antitumor agents to the kidney. Se-substituted selenocysteine conjugates may be more promising prodrugs because these are much better substrates for .beta.-lyase.

L15 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Chemical form of selenium, critical metabolites, and cancer prevention

AN 1991:135663 CAPLUS

DN 114:135663

TI Chemical form of selenium, critical metabolites, and cancer prevention

AU Ip, Clement; Hayes, Cassandra; Budnick, Rose Marie; Ganther, Howard E.

CS Dep. Breast Surg., Roswell Park Cancer Inst., Buffalo, NY, 14263, USA

SO Cancer Research (1991), 51(2), 595-600

CODEN: CNREA8; ISSN: 0008-5472

DT Journal

LA English

AB Methylated selenides are prominent metabolites at the dietary levels used for obtaining anticarcinogenic effects with selenium. The present study reports the chemopreventive activities of 2 novel selenium compds. Se-methylselenocysteine and di-Me selenoxide, in the rat dimethylbenz(a)anthracene-induced mammary tumor model. Other treatment groups were supplemented with either selenite or selenocystine for comparative purposes. Each selenium compd. was tested at different levels and was given to the animal starting 1 wk before dimethylbenz(a)anthracene administration and continued until sacrifice. Results of the carcinogenesis expts. showed that the relative efficacy with the four compds. was Se-methylselenocysteine > selenite > selenocystine > di-Me selenoxide. In correlating the chem. form and metab. of these selenium compds. with their anticarcinogenic activity, it is concluded that: (a) selenium compds. that are able to generate a steady stream of methylated metabolites, particularly the monomethylated species, are likely to have good chemopreventive potential; (b) anticarcinogenic activity is lower for selenoamino acids, such as selenocysteine following conversion from selenocystine, which have an escape mechanism via random, nonstoichiometric incorporation into proteins; and (c) forms of selenium, as exemplified by dimethylselenoxide, which are metabolized rapidly and quant. to di-Me selenide and trimethylselenonium and excreted, are likely to be poor choices. A sep. bioavailability study using Se-methylselenocysteine, di-Me selenoxide, and trimethylselenonium as the starting compds. for delivering selenium with one, two, or three Me groups was undertaken and the ability of these compds. to restore glutathione peroxidase activity in selenium-depleted animals was measured. All three compds. were able to fully replete this enzyme, although with a wide range of efficiency (Se-methylselenocysteine > dimethyl selenoxide > trimethylselenonium), suggesting that complete demethylation to inorg. selenium is a normal process of selenium metab. However, the degree to which this occurs under chemoprevention conditions would argue against the involvement of selenoproteins in the anticarcinogenic action of these selenium compds.

L15 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Preparation of sulfur and selenium amino acids with microbial pyridoxal phosphate enzymes

AN 1988:128044 CAPLUS

DN 108:128044

TI Preparation of sulfur and selenium amino acids with microbial pyridoxal phosphate enzymes

AU Esaki, Nobuyoshi; Soda, Kenji

CS Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan

SO Methods in Enzymology (1987), 143(Sulfur Sulfur Amino Acids), 291-7

CODEN: MENZAU; ISSN: 0076-6879

DT Journal

LA English  
 AB The prepn. of S-substituted L-homocysteines with L-methionine .gamma.-lyase (I), S-substituted L-cysteines and Se-substituted L-selenocysteines with tryptophan synthase, L-selenocystine and -homocystine with O-acetylhomoserine sulphydrylase, and deuterated and tritiated L-methionine and S-methyl-L-cysteine with I are illustrated.

L15 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Selenium-containing amino acids  
 AN 1984:4789 CAPLUS  
 DN 100:4789  
 TI Selenium-containing amino acids  
 PA Mitsui Toatsu Chemicals, Inc., Japan  
 SO Jpn. Kokai Tokkyo Koho, 3 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 58146286	A2	19830831	JP 1982-28108	19820225
	JP 02054076	B4	19901120		

JP 1982-28108 19820225

AB A compn. contg. methaneselenol [6486-05-1] or benzylselenol [16645-12-8] and L-serine [56-45-1] is treated with tryptophan synthetase [9014-52-2] to produce Se-methylselenocysteine [26046-90-2] or Se-benzylselenocysteine [2575-74-8]. Thus, a compn. contg. L-serine 30, methaneselenol 50, pyridoxal phosphate 0.01 mM, and tryptophan synthetase 10 mg/dL was shaken at 30.degree. for 24 h. The medium contained Se-methylselenocysteine with a mol. yield rate of 28%.

L15 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Enzymatic synthesis of selenium-substituted L-selenocysteine with tryptophan synthase  
 AN 1983:590469 CAPLUS  
 DN 99:190469  
 TI Enzymatic synthesis of selenium-substituted L-selenocysteine with tryptophan synthase  
 AU Esaki, Nobuyoshi; Tanaka, Hidehiko; Miles, Edith W.; Soda, Kenji  
 CS Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan  
 SO FEBS Letters (1983), 161(2), 207-9  
 CODEN: FEBLAL; ISSN: 0014-5793

DT Journal  
 LA English  
 AB When L-serine was incubated with the purified .alpha.2.beta.2 complex of tryptophan synthase (EC 4.2.1.20) from Escherichia coli in the presence of a std. reaction mixt. contg. .alpha.-tolueneselenol, Se-benzyl-L-5-selenocysteine was formed with a yield of 44%, based on the L-serine used. The product was identified by several physicochem. criteria, including NMR. L-Serine was also converted to Se-methyl-L-selenocysteine by this method with methaneselenol as a reactant. The yield was 16%, based on L-serine. The reactivities of selenols were compared to those of thiols in a reaction system in which L-serine was used as a substrate. The specific activities of tryptophan synthase in .beta.-replacement reactions with .alpha.-tolueneselenol and methaneselenol were 0.96 and 0.77, resp., whereas those with .alpha.-toluenethiol and methanethiol were 3.2 and 0.61, resp. Possible reasons for these reactivities are discussed.

L15 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS on STN

TI Selenoamino acids  
 AN 1979:522166 CAPLUS  
 DN 91:122166  
 TI Selenoamino acids

IN Sayuda, Kenji; Tanaka, Hidehiko  
 PA Ajinomoto Co., Inc., Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 54052033	A2	19790424	JP 1977-117664	19770929
	JP 57008717	B4	19820217		
				JP 1977-117664	19770929

AB Eight selenoamino acids  $RSe(CH_2)_nCH(NH_2)CO_2H$  ( $R$  = org. residues;  $n$  = 1, 2) were prepd. by reaction of  $R_1(CH_2)_nCH(NH_2)CO_2H$  [ $R_1$  = halo,  $R_2O$  ( $R_2$  = H, alkyl),  $R_2S$ ,  $R_2SO$ ,  $R_2SO_2$ ] with  $RSeH$  in aq. media in the presence of methioninase. Thus, *Pseudomonas ovalis* IFO 3738 was cultured on 1 kg of broth (pH 7.2) contg. L-methionine 0.25, urea 0.1, peptone 0.1, glycerol 0.1,  $KH_2PO_4$  0.1,  $K_2HPO_4$  0.1,  $MgSO_4 \cdot 7H_2O$  0.01, and yeast ext. 0.025 g/dL 18 h at 28.degree. to give 2.2 kg cells, which were crushed in  $H_3PO_4$  buffer and the supernatant treated on DEAE-cellulose and Sephadex G-200 to give 280 mg enzyme protein. A mixt. of 0.1M L-methionine (in 0.2M  $H_3PO_4$  buffer at pH 8.0), 0.1 mL 1M PhSeH (in EtOH), 0.5 mL 10-5M pyridoxal phosphate (in 0.02M  $H_3PO_4$  buffer at pH 8.0), and 1 mL of the enzyme liq. (50 .mu.g of protein/mL) was kept for 2 h at 37.degree. under N with addn. of 3 .times. 200 .mu.L of the enzyme liq. and 3 .times. 100 .mu.L the PhSeH liq. and the whole kept 25 min at 100.degree. to give 4.3 mg .gamma.-phenylseleno-.alpha.-aminobutyric acid [71128-79-5].

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	32.67	72.45
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.51	-7.16

FILE 'REGISTRY' ENTERED AT 12:12:20 ON 08 OCT 2003  
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STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2  
 DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNnote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 10065677 lgalananine me ester.str

L16        STRUCTURE UPLOADED

=> d 116

L16 HAS NO ANSWERS

L16                STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search 116 sss sam

SAMPLE SEARCH INITIATED 12:12:51 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1801 TO ITERATE

55.5% PROCESSED        1000 ITERATIONS

2 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:            33475 TO        38565

PROJECTED ANSWERS:                2 TO            185

L17                2 SEA SSS SAM L16

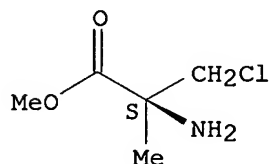
=> d scan

L17 2 ANSWERS    REGISTRY    COPYRIGHT 2003 ACS on STN

IN    D-Alanine, 3-chloro-2-methyl-, methyl ester, hydrochloride (9CI)

MF    C5 H10 Cl N O2 . Cl H

Absolute stereochemistry.



● HCl

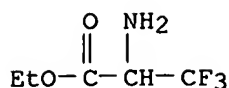
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L17 2 ANSWERS    REGISTRY    COPYRIGHT 2003 ACS on STN

IN    Alanine, 3,3,3-trifluoro-, ethyl ester, hydrochloride (9CI)

MF    C5 H8 F3 N O2 . Cl H





● HCl

ALL ANSWERS HAVE BEEN SCANNED

=> search l16 sss full  
 FULL SEARCH INITIATED 12:13:26 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 35539 TO ITERATE

100.0% PROCESSED 35539 ITERATIONS 287 ANSWERS  
 SEARCH TIME: 00.00.01

L18 287 SEA SSS FUL L16

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	148.55	221.00
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.16

FILE 'CAPLUS' ENTERED AT 12:13:32 ON 08 OCT 2003  
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FILE COVERS 1907 - 8 Oct 2003 VOL 139 ISS 15  
 FILE LAST UPDATED: 7 Oct 2003 (20031007/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:56:41 ON 08 OCT 2003)

FILE 'STNGUIDE' ENTERED AT 11:56:53 ON 08 OCT 2003

FILE 'HOME' ENTERED AT 11:57:00 ON 08 OCT 2003

FILE 'STNGUIDE' ENTERED AT 11:57:05 ON 08 OCT 2003

FILE 'CAPLUS' ENTERED AT 11:57:35 ON 08 OCT 2003  
ACT CHLOROALA/A

-----  
L1 STR  
L2 ( 4)SEA FILE=REGISTRY EXA FUL L1  
L3 14 SEA FILE=CAPLUS ABB=ON PLU=ON L2  
-----

ACT MESEALA/A  
-----  
L4 STR  
L5 ( 102)SEA FILE=REGISTRY SSS FUL L4  
L6 241 SEA FILE=CAPLUS ABB=ON PLU=ON L5  
-----

FILE 'REGISTRY' ENTERED AT 11:58:15 ON 08 OCT 2003  
E DIMETHYLDISELENIDE/CN  
E DIMETHYL DISELENIDE/CN  
L7 2128 \E3  
L8 2128 \E3  
L9 1 E3  
E METHYL SELENOL  
E METHYL SELENOL/CN  
E METHYL SELENIDE/CN  
L10 1 E3

FILE 'CAPLUS' ENTERED AT 12:00:49 ON 08 OCT 2003  
L11 356 L9  
L12 8 L11 AND L6

FILE 'REGISTRY' ENTERED AT 12:06:03 ON 08 OCT 2003  
E L-SE-METHYLSELENOCYSTEINE/CN  
E METHYLSELENOCYSTEINE/CN  
L13 2 E3

FILE 'CAPLUS' ENTERED AT 12:07:01 ON 08 OCT 2003  
L14 112 L13  
L15 10 L13/PREP

FILE 'REGISTRY' ENTERED AT 12:12:20 ON 08 OCT 2003  
L16 STRUCTURE UPLOADED  
L17 2 SEARCH L16 SSS SAM  
L18 287 SEARCH L16 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:13:32 ON 08 OCT 2003

=> l18 and l14  
260 L18  
L19 0 L18 AND L14

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.75	224.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.16

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 12:19:02 ON 08 OCT 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 12:57:33 ON 08 OCT 2003  
FILE 'CAPLUS' ENTERED AT 12:57:33 ON 08 OCT 2003  
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.75	224.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.16
=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.75	224.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.16

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 12:57:46 ON 08 OCT 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 13:15:28 ON 08 OCT 2003  
FILE 'CAPLUS' ENTERED AT 13:15:28 ON 08 OCT 2003  
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.75	224.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.16
=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.42	226.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.16

FILE 'REGISTRY' ENTERED AT 13:17:38 ON 08 OCT 2003  
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STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2  
 DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e selenocysteine/cn

E1	1	SELENOCYSTEAMINE/CN
E2	1	SELENOCYSTEIC ACID/CN
E3	1 -->	SELENOCYSTEINE/CN
E4	1	SELENOCYSTEINE .BETA.-LYASE/CN
E5	1	SELENOCYSTEINE INSERTION SEQUENCE BINDING PROTEIN 2 (HUMAN C LONE A11)/CN
E6	1	SELENOCYSTEINE LYASE/CN
E7	1	SELENOCYSTEINE LYASE (AMINOTRANSFERASE OF NIFS FAMILY) (CLOS TRIDIUM ACETOBUTYLICUM STRAIN ATCC 824 GENE CAC2805)/CN
E8	1	SELENOCYSTEINE LYASE (BLOCHMANNIA FLORIDANUS GENE SUFS)/CN
E9	1	SELENOCYSTEINE LYASE (COXIELLA BURNETII STRAIN RSA 493 GENE CSDB)/CN
E10	1	SELENOCYSTEINE LYASE (ESCHERICHIA COLI CFT073 STRAIN CFT073 GENE C2075)/CN
E11	1	SELENOCYSTEINE LYASE (ESCHERICHIA COLI STRAIN O157:H7 GENE E CS2387)/CN
E12	1	SELENOCYSTEINE LYASE (HUMAN CLONE MGC:3039 IMAGE:3163969)/CN

=> e3

L20 1 SELENOCYSTEINE/CN

=> d 120

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN

RN 3614-08-2 REGISTRY

CN Alanine, 3-selenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-Selenyl-DL-alanine

CN DL-Selenocysteine

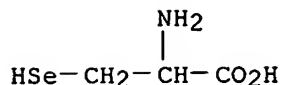
CN **Selenocysteine**

DR 18312-66-8

MF C3 H7 N O2 Se

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CEN, CIN, EMBASE, HSDB\*, NIOSHTIC, PROMT, RTECS\*, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)



498 REFERENCES IN FILE CA (1907 TO DATE)  
21 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
498 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

6.30	232.72
------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-7.16
------	-------

FILE 'CAPLUS' ENTERED AT 13:18:10 ON 08 OCT 2003  
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FILE COVERS 1907 - 8 Oct 2003 VOL 139 ISS 15  
FILE LAST UPDATED: 7 Oct 2003 (20031007/ED)

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=> 120

L21 500 L20

=> 120/prep

500 L20  
3060787 PREP/RL  
L22 24 L20/PREP  
(L20 (L) PREP/RL)

=> d 122 20-24 ti

L22 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Organoselenium chemistry. Alkylation of acid, ester, amide, and ketone enolates with bromomethyl benzyl selenide and sulfide. Preparation of selenocysteine derivatives

L22 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN

TI Synthesis of L-selenodjenkolate and its degradation with methionine  
.gamma.-lyase

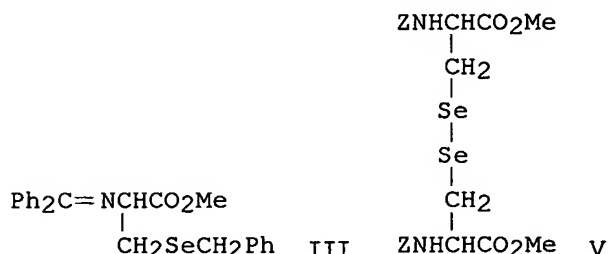
L22 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Somatostatin and somatostatin analog

L22 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Usefulness of N-ethylmaleimide in the identification of 75Se-labeled  
selenocysteine

L22 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Synthesis of selno-amino acids in cell-free extracts of Candida albicans

=> d 122 20 ti fbib abs

L22 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Organoselenium chemistry. Alkylation of acid, ester, amide, and ketone  
enolates with bromomethyl benzyl selenide and sulfide. Preparation of  
selenocysteine derivatives  
AN 1986:460921 CAPLUS  
DN 105:60921  
TI Organoselenium chemistry. Alkylation of acid, ester, amide, and ketone  
enolates with bromomethyl benzyl selenide and sulfide. Preparation of  
selenocysteine derivatives  
AU Reich, Hans J.; Jasperse, Craig P.; Renga, James M.  
CS Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA  
SO Journal of Organic Chemistry (1986), 51(15), 2981-8  
CODEN: JOCEAH; ISSN: 0022-3263  
DT Journal  
LA English  
OS CASREACT 105:60921  
GI



AB Bromomethyl benzyl selenide (I) was prepd. and used for the alkylation of  
carboxylic acid and amide dianions and ketones and ester enolates. Thus,  
PhCH<sub>2</sub>CO<sub>2</sub>H was alkylated with I in the presence of LDA to give  
PhCH<sub>2</sub>SeCH<sub>2</sub>CHPhCO<sub>2</sub>H. Clean reaction could not be achieved for ketones and  
esters whose alkylation products were subject to selenolate elimination.  
I reacted 18 times more slowly than bromomethyl benzyl sulfide (II), which  
alkylated ketones in fair yield even in cases where the selenide failed.  
The II alkylation products gave .alpha.-methylene ketones upon oxidn. to  
sulfoxide and thermolysis. Protected amino acid enolates (valine,  
alanine, and glycine) were alkylated with I. Thus, glycine deriv.  
Ph<sub>2</sub>C:NCH<sub>2</sub>CO<sub>2</sub>Me was alkylated with I to give selenide III. III was  
N-cleaved and then acylated with PhCH<sub>2</sub>O<sub>2</sub>CCl (ZCl) to give  
PhCH<sub>2</sub>SeCH<sub>2</sub>CH(NHZ)CO<sub>2</sub>Me (IV), which was oxidized by m-CPBA to give  
ZNHC(:CH<sub>2</sub>)CO<sub>2</sub>Me. IV was cleaved by Br<sub>2</sub> and then treated with NH<sub>2</sub>NH<sub>2</sub> to  
give selenocystine V. Halogen reagents (Br<sub>2</sub>, SO<sub>2</sub>Cl<sub>2</sub>) were shown to very  
efficiently and generally convert benzyl selenides to selenenyl halides,

which were converted to diselenides or selenides by redn. or alkylolation.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
9.00	241.72

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.65	-7.81

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:22:45 ON 08 OCT 2003

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Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS	5	Jul 21	Identification of STN records implemented
NEWS	6	Jul 21	Polymer class term count added to REGISTRY
NEWS	7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS	8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS	11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS	12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS	13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS	14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS	17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	18	SEP 22	DIPPR file reloaded
NEWS	19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	20	SEP 29	DISSABS now available on STN
NEWS EXPRESS		OCTOBER 01	CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS			STN Operating Hours Plus Help Desk Availability

NEWS INTER      General Internet Information  
 NEWS LOGIN     Welcome Banner and News Items  
 NEWS PHONE     Direct Dial and Telecommunication Network Access to STN  
 NEWS WWW       CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 08:25:06 ON 09 OCT 2003

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'STNGUIDE' ENTERED AT 08:25:18 ON 09 OCT 2003

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 AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Oct 3, 2003 (20031003/UP).

=> DIS SAVED

NAME	CREATED	NOTES/TITLE
ACRYLMETATH/A	TEMP	67 ANSWERS IN FILE CAPLUS
ALKYLATIN/L	13 DEC 2001	9 L-NUMBERS
CHLOROALA/A	TEMP	14 ANSWERS IN FILE CAPLUS
ESTERODOR/L	05 SEP 2002	42 L-NUMBERS
HYDROXAMINES/A	TEMP	8641 ANSWERS IN FILE CAPLUS
INDIUMCL3/A	30 MAY 2001	1 ANSWER IN FILE REGISTRY
LTWENTAUGFOR/A	04 AUG 2001	72 ANSWERS IN FILE CAPLUS
MESEALA/A	TEMP	241 ANSWERS IN FILE CAPLUS
METATHESIS/L	TEMP	36 L-NUMBERS
METHIDES/A	TEMP	500 ANSWERS IN FILE CAPLUS
NEOTAMECRYST/A	24 APR 2001	59 ANSWERS IN FILE CAPLUS
NVLARMFULGEN/A	19 APR 2001	196 ANSWERS IN FILE REGISTRY
POHBENZALDEH/A	10 JUL 2001	5519 ANSWERS IN FILE CAPLUS
POLYINHBT/L	TEMP	15 L-NUMBERS
PROSTACMPD15/A	01 AUG 2001	34 ANSWERS IN FILE CAPLUS
SELENOCMPDS/L	TEMP	13 L-NUMBERS
STILLEAPP/L	07 JAN 2002	17 L-NUMBERS
TWOAMINOPOLY/Q	16 APR 2001	UPLOADED STRUCTURE

=> DIS SAVED/S

NO SAVED SDI REQUESTS

=> FIL HOME

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.06	0.27



FILE 'HOME' ENTERED AT 08:25:59 ON 09 OCT 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.48

FILE 'REGISTRY' ENTERED AT 08:26:08 ON 09 OCT 2003

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STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e methylselenocysteine/cn

E1	1	METHYLSELENOCYANATE/CN
E2	1	METHYLSELENOCYANIDE/CN
E3	2 -->	METHYLSELENOCYSTEINE/CN
E4	1	METHYLSELENOL/CN
E5	1	METHYLSELENOMAGNESIUM BROMIDE/CN
E6	1	METHYLSELENOMAGNESIUM IODIDE/CN
E7	1	METHYLSELENOMETHIONINE/CN
E8	1	METHYLSELENOMETHYLLITHIUM/CN
E9	1	METHYLSELENYL CHLORIDE/CN
E10	1	METHYLSELENOCHOLINE/CN
E11	1	METHYLSEMISSQUARIC ACID ION(1-)/CN
E12	1	METHYLSILAISONITRILE/CN

=> e3

L1 2 METHYLSELENOCYSTEINE/CN

=> d l1 1-2

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN

RN 26046-90-2 REGISTRY

CN L-Alanine, 3-(methylseleno)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Alanine, 3-(methylselenyl)-, L- (8CI)

OTHER NAMES:

CN 3-(Methylseleno)-L-alanine

CN Methylseleno-L-cysteine

CN **Methylselenocysteine**

CN Se-Methylselenocysteine

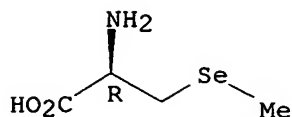
FS STEREOSEARCH

MF C4 H9 N O2 Se

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, DDFU, DRUGU, TOXCENTER, USPATFULL

(\*File contains numerically searchable property data)

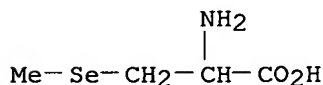
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

80 REFERENCES IN FILE CA (1907 TO DATE)  
80 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 2574-71-2 REGISTRY  
CN Alanine, 3-(methylseleno)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, 3-(methylselenyl)- (6CI, 7CI, 8CI)  
OTHER NAMES:  
CN DL-Se-methylselenocysteine  
CN **Methylselenocysteine**  
CN NSC 319053  
CN Selenocysteine, Se-methyl-  
DR 26145-42-6  
MF C4 H9 N O2 Se  
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CANCERLIT, CAOLD,  
CAPLUS, CHEMCATS, MEDLINE, TOXCENTER  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

34 REFERENCES IN FILE CA (1907 TO DATE)  
34 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	8.38	8.86

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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15  
FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 11

L2 112 L1

=> amine

238970 AMINE

229162 AMINES

L3 367971 AMINE

(AMINE OR AMINES)

=> 12 and 13

L4 2 L2 AND L3

=> d 14 1-2 ti fbib abs

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

TI Changes in ornithine decarboxylase activity and polyamine levels in response to eight different forms of selenium

AN 1992:53105 CAPLUS

DN 116:53105

TI Changes in ornithine decarboxylase activity and polyamine levels in response to eight different forms of selenium

AU Thompson, H. J.; Ip, C.; Ganther, H. E.

CS Lab. Nutr. Res., AMC Cancer Res. Cent., Denver, CO, 80214, USA

SO Journal of Inorganic Biochemistry (1991), 44(4), 283-92

CODEN: JIBIDJ; ISSN: 0162-0134

DT Journal

LA English

AB The biol. activity of selenium is known to depend on its chem. form. In this study, eight forms of selenium that differed in oxidn. state or degree of methylation were studied for their acute effects on the activities of ornithine decarboxylase (ODC) and S-adenosylmethionine decarboxylase (AdoMet DC) and on the concns. of the polyamines putrescine, spermidine, and spermine in the liver. The polyamine pathway was studied because it is involved in the control of cell growth and in the cell's response to trophic, carcinogenic, and toxic stimuli, activities that selenium has been reported to affect. Female Sprague Dawley rats were administered 12 .mu.mol Se/kg via i.p. injection and were sacrificed six h later. Injection of sodium selenate, sodium selenite, selenomethionine, Se-methylselenocysteine, selenobetaine, and selenobetaine Me ester resulted in significant increases in liver selenium, whereas injection and dimethylselenoxide and trimethylselenonium chloride did not. ODC activity and AdoMet DC activity were induced by those selenium compds. that also increased liver selenium content, but the magnitude of enzyme induction by those compds. was not correlated with the hepatic concn. of total selenium detd. fluorometrically. Furthermore, the induction of ODC activity by the various forms of selenium did not result in concomitant increases in putrescine, spermidine, and spermine except in the case of selenite. Given that alterations in the metab. of selenium are induced when the level of tissue selenium is evaluated and that the relative abundance of various selenometabolites can be affected by the point of entry of selenium into intermediary metab., these data suggest that the changes that were obsd. in enzyme activities and polyamine levels are likely to be

assocd. with the accumulation of a specific metabolite of selenium.

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN  
TI The C3-N bond cleavage of 2-amino-3-(N-substituted-amino)-propionic acids  
catalyzed by L-methionine .gamma.-lyase  
AN 1989:91177 CAPLUS  
DN 110:91177  
TI The C3-N bond cleavage of 2-amino-3-(N-substituted-amino)-propionic acids  
catalyzed by L-methionine .gamma.-lyase  
AU Takada, Harumi; Esaki, Nobuyoshi; Tanaka, Hidehiko; Soda, Kenji  
CS Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan  
SO Agricultural and Biological Chemistry (1988), 52(11), 2897-901  
CODEN: ABCHA6; ISSN: 0002-1369  
DT Journal  
LA English  
AB L-Methionine .gamma.-lyase (EC 4.4.1.11) catalyzes .alpha., .beta.-  
elimination of L-2-amino-3-(N-methylamino)propionic acid and  
L-2-amino-3-(N-hydroxyethylamino)propionic acid to yield pyruvate, NH3,  
and the corresponding amines. These amino acids also undergo  
the enzymic .beta.-replacement reaction with thiols to produce the  
corresponding S-substituted cysteines. Thus, L-methionine .gamma.-lyase  
cleaves a C-N bond in addn. to C-S, C-Se, and C-O bonds at the .beta.  
position of amino acids by elimination and replacement reactions. A  
linear relationship between the reactivity, (Vmax/Km) and the pKa value of  
the conjugated acid of the leaving group has been found for  
Se-methyl-L-selenocysteine, S-methyl-L-cysteine, and O-methyl-L-serine.  
However, L-2-amino-3-(N-methylamino)propionic acid has shown lower  
reactivity than that expected from the pKa value of methylammonium ions.

=> racemiz? or racemis?  
35 RECEMIZ?  
31 RACEMIS?  
L5 66 RECEMIZ? OR RACEMIS?

=> racemiz? or racemis?  
10416 RACEMIZ?  
31 RACEMIS?  
L6 10436 RACEMIZ? OR RACEMIS?

=> d his

(FILE 'HOME' ENTERED AT 08:25:06 ON 09 OCT 2003)

FILE 'STNGUIDE' ENTERED AT 08:25:18 ON 09 OCT 2003

FILE 'HOME' ENTERED AT 08:25:59 ON 09 OCT 2003

FILE 'REGISTRY' ENTERED AT 08:26:08 ON 09 OCT 2003  
E METHYLSELENOCYSTEINE/CN

L1 2 E3

FILE 'CAPLUS' ENTERED AT 08:27:04 ON 09 OCT 2003

L2 112 L1  
L3 367971 AMINE  
L4 2 L2 AND L3  
L5 66 RECEMIZ? OR RACEMIS?  
L6 10436 RACEMIZ? OR RACEMIS?

=> 12 and 16

L7 0 L2 AND L6

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	16.78	25.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-1.30	-1.30

FILE 'CAPLUS' ENTERED AT 08:31:56 ON 09 OCT 2003  
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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15  
 FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> e cysteine/cn

# **REGISTRY INITIATED**

Substance data EXPAND from CAS REGISTRY in progress...

E1	1	CYSTEINAMINE DISULFIDE/CN
E2	1	CYSTEINAMINE HYDROCHLORIDE/CN
E3	2 -->	CYSTEINE/CN
E4	1	CYSTEINE -- TRNA LIGASE (PLASMODIUM FALCIPARUM STRAIN 3D7 GE NE PF10-0149)/CN
E5	1	CYSTEINE ABC TRANSPORTER, ATP-BINDING PROTEIN (PSEUDOMONAS P UTIDA STRAIN KT2440 GENE PP0225)/CN
E6	1	CYSTEINE ABC TRANSPORTER, PERIPLASMIC CYSTEINE-BINDING PROTE IN (PSEUDOMONAS PUTIDA STRAIN KT2440 GENE PP0227)/CN
E7	1	CYSTEINE ABC TRANSPORTER, PERMEASE PROTEIN (PSEUDOMONAS PUTI DA STRAIN KT2440 GENE PP0226)/CN
E8	1	CYSTEINE ACETATE/CN
E9	1	CYSTEINE ACRYLAMIDE-METHYLENEBISACRYLAMIDE COPOLYMER/CN
E10	1	CYSTEINE AMINOPEPTIDASE (LACTOBACILLUS DELBURECKII LACTIS DS M7290)/CN
E11	1	CYSTEINE AMINOPEPTIDASE (LACTOBACILLUS PLANTARUM STRAIN WCFS 1 GENE PEPC1)/CN
E12	1	CYSTEINE AMINOPEPTIDASE (LACTOBACILLUS PLANTARUM STRAIN WCFS 1 GENE PEPC2)/CN

=> e3

# **REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L9 33224 L8

=> 16 and 19

L10 86 L6 AND L9

=> 16(1)19

L11 26 L6(L)L9

=> benzaldehyde

60733 BENZALDEHYDE

5839 BENZALDEHYDES

L12 62938 BENZALDEHYDE  
(BENZALDEHYDE OR BENZALDEHYDES)

=> 111 and 112

L13 0 L11 AND L12

=> 110 and 112

L14 2 L10 AND L12

=> d 114 1-2 ti

L14 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

TI Application of chiral thiazolidine ligands to asymmetric hydrosilation

L14 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

TI Chemical determination of tryptophan in proteins

=> aldehyde

94231 ALDEHYDE

91091 ALDEHYDES

L15 146703 ALDEHYDE  
(ALDEHYDE OR ALDEHYDES)

=> 111 and 115

L16 1 L11 AND L15

=> d 116 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

TI Free L-.alpha.-amino acids

AN 1984:7156 CAPLUS

DN 100:7156

TI Free L-.alpha.-amino acids

IN Commeyras, Auguste; Previero, Aldo; Pugnieri, Martine

PA Centre National de la Recherche Scientifique, Fr.; Institut National de la  
Sante et de la Recherche Medicale (INSERM)

SO Eur. Pat. Appl., 33 pp.

CODEN: EPXXDW

DT Patent

LA French

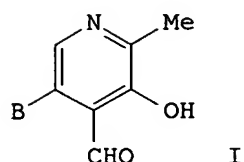
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	EP 89886	A1	19830928	EP 1983-400546	19830316
	EP 89886	B1	19881012		

R: AT, BE, CH, DE, GB, IT, LI, LU, NL, SE

FR 2523961	A1	19830930	FR 1982-4886	19820323
FR 2523961	B1	19850830	FR 1982-4886	19820323
US 4540792	A	19850910	US 1983-472479	19830307
			FR 1982-4886	19820323
AT 37861	E	19881015	AT 1983-400546	19830316
			FR 1982-4886	19820323
			EP 1983-400546	19830316
JP 59002694	A2	19840109	JP 1983-47312	19830323
			FR 1982-4886	19820323

GI



AB L-.alpha.-Amino acids were prepd. from D-.alpha.-amino acid esters. The D-.alpha.-amino acid esters underwent catalytic racemization to produce an equil. mixt. of D- and L-.alpha.-amino acid esters, and the resulting L-ester underwent preferential enzymic hydrolysis to give the L-.alpha.-amino acids. The racemization catalysts were arom. **aldehydes** contg. a basic function; preferentially a pyridoxal related compd. Thus, a 0.510 .times. 10<sup>-2</sup> M aq. soln. of pyridoxal 5'-phosphate was supported on DEAE-cellulose at pH 7 and 20.degree., 10<sup>-2</sup> M D-tyrosine Me ester was added, the suspension was stirred at 20.degree., and then chymotrypsin was added to give L-tyrosine (50% after 160 min).

=>

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
18.98	50.48

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.65	-1.95

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:50:26 ON 09 OCT 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

SESSION RESUMED IN FILE 'CAPLUS' AT 08:59:48 ON 09 OCT 2003

FILE 'CAPLUS' ENTERED AT 08:59:48 ON 09 OCT 2003

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
------------	-------

FULL ESTIMATED COST	ENTRY 18.98	SESSION 50.48
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY -0.65	SESSION -1.95

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY 18.98	SESSION 50.48
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY -0.65	SESSION -1.95

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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15  
 FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

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=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY 0.42	SESSION 50.90
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -1.95

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2  
 DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.



Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e serine/cn

E1	1	SERINAMIDE, P-TOLUENESULFONATE/CN
E2	1	SERINAMIDE, P-TOLUENESULFONATE, HYDROBROMIDE/CN
E3	2 -->	SERINE/CN
E4	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE A (ALPHA-1 ANTIPROTEINASE, ANTITRYPSIN), MEMBER 10 (HUMAN CLONE MGC:22287 IMAGE:4710734)/CN
E5	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE A (ALPHA-1 ANTIPROTEINASE, ANTITRYPSIN), MEMBER 3 (HUMAN CLONE MGC:18107 IMAGE:4152390)/CN
E6	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE A (ALPHA-1 ANTIPROTEINASE, ANTITRYPSIN), MEMBER 3 (HUMAN CLONE MGC:1813 IMAGE:3547133)/CN
E7	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 1 (HUMAN CLONE MGC:9340 IMAGE:3456154)/CN
E8	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 1B (MOUSE CLONE MGC:40788 IMAGE:5367365)/CN
E9	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 3 (HUMAN CLONE MGC:12244 IMAGE:4101988)/CN
E10	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 5 (MOUSE STRAIN FVB/N CLONE MGC:5950 IMAGE:3600282)/CN
E11	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 6 (HUMAN CLONE MGC:2180 IMAGE:3051381)/CN
E12	1	SERINE (OR CYSTEINE) PROTEINASE INHIBITOR, CLADE B (OVALBUMIN), MEMBER 6 (MOUSE STRAIN C57BL/6J CLONE MGC:6042 IMAGE:3481963)/CN

=> e3

L17 2 SERINE/CN

=> e thionyl chloride/cn

E1	1	THIONYL BROMIDE, COMPD. WITH QUINOLINE (1:2)/CN
E2	1	THIONYL BROMIDE, COMPD. WITH QUINOLINE (2:1)/CN
E3	1 -->	THIONYL CHLORIDE/CN
E4	1	THIONYL CHLORIDE (SOCL2)/CN
E5	1	THIONYL CHLORIDE COMPD. WITH METHYL BENZOATE (1:2)/CN
E6	1	THIONYL CHLORIDE COMPOUND WITH DIMETHYLFORMAMIDE (1:2)/CN
E7	1	THIONYL CHLORIDE COMPOUND WITH DIMETHYLFORMAMIDE (1:3)/CN
E8	1	THIONYL CHLORIDE CYANIDE/CN
E9	1	THIONYL CHLORIDE FLUORIDE/CN
E10	1	THIONYL CHLORIDE HYDRIDE/CN
E11	1	THIONYL CHLORIDE NITRATE/CN
E12	5	THIONYL CHLORIDE, ALUMINUM COMPLEX/CN

=> e3

L18 1 "THIONYL CHLORIDE"/CN

=> e thionyl bromide/cn

E1	1	THIONUPHLUTINE C/CN
E2	1	THIONUPHLUTINE C DIMETHIODIDE/CN
E3	1 -->	THIONYL BROMIDE/CN
E4	1	THIONYL BROMIDE CHLORIDE/CN
E5	1	THIONYL BROMIDE FLUORIDE/CN
E6	1	THIONYL BROMIDE HYDRIDE ((SO)BRH)/CN

E7	1	THIONYL BROMIDE, BORON COMPLEX/CN
E8	1	THIONYL BROMIDE, BORON DERIV./CN
E9	1	THIONYL BROMIDE, COMPD. WITH 2-PICOLINE (1:1)/CN
E10	1	THIONYL BROMIDE, COMPD. WITH 2-PICOLINE (1:2)/CN
E11	1	THIONYL BROMIDE, COMPD. WITH 2-PICOLINE (2:1)/CN
E12	1	THIONYL BROMIDE, COMPD. WITH 3-PICOLINE (1:2)/CN

=> e3

L19 1 "THIONYL BROMIDE"/CN

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.46	64.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.95

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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15  
 FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 117

L20 31363 L17

=> 118

L21 5368 L18

=> 119

L22 194 L19

=> 121 or 122

L23 5444 L21 OR L22

=> 120 and 123

L24 6 L20 AND L23

=> d 124 1-6 ti fbib abs

L24 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
 TI Structure-function analysis of lipopeptide pheromones from the plant pathogen Ustilago maydis  
 AN 2002:870632 CAPLUS

DN 139:194264  
TI Structure-function analysis of lipopeptide pheromones from the plant  
pathogen *Ustilago maydis*  
AU Szabo, Z.; Toennis, M.; Kessler, H.; Feldbruegge, M.  
CS Inst. Genet. Microbiol., Ludwig Maximilians Univ. Munich, Munchen, 80638,  
Germany  
SO Molecular Genetics and Genomics (2002), 268(3), 362-370  
CODEN: MGGOAA; ISSN: 1617-4615

PB Springer-Verlag

DT Journal

LA English

AB Mating of 2 haploid cells is a prerequisite for the successful infection of corn by the pathogenic fungus *U. maydis*. Cell-cell recognition is mediated by small lipopeptide pheromones. Genes encoding pheromone precursors as well as pheromone receptors are located in the a mating type locus. Two pheromones are known, the tridecapeptide a1 and the nonapeptide a2, both of which contain an S-prenylated cysteine Me ester at the C-terminus. It has previously been shown that synthetic pheromones are active in a biol. test system. Here, we used the same assay to perform a detailed anal. of synthetic a1 and a2 pheromones. Testing of truncated derivs. of a1 and a2 revealed that in both cases the pheromone function is less sensitive to N-terminal than to C-terminal truncations. Replacement of each amino acid in the a1 pheromone by either alanine or the corresponding D-amino acids revealed that 4 positions are important for function: the 2 central glycines (positions 5 and 9), proline at position 7, and tyrosine at position 10. By introducing different naturally occurring as well as synthetic amino acids at position 10, we demonstrate that the presence of an arom. side chain at this position is necessary for function. We propose a model in which a cis peptide bond at proline 7 favors the formation of a type II' .beta. turn of the a1 pheromone backbone with glycine 9 in position i+1 (where i refers to the 1st position of the .beta. turn). As a result, tyrosine 10, at position i+2 of the turn, would be highly exposed and could be inserted into a structurally well-defined binding pocket of the receptor. The latter may represent an important facet of receptor specificity.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
TI 13C Gas Chromatography-Combustion Isotope Ratio Mass Spectrometry Analysis of N-Pivaloyl Amino Acid Esters of Tissue and Plasma Samples  
AN 2000:87593 CAPLUS  
DN 132:331624  
TI 13C Gas Chromatography-Combustion Isotope Ratio Mass Spectrometry Analysis of N-Pivaloyl Amino Acid Esters of Tissue and Plasma Samples  
AU Metges, Cornelia C.; Daenzer, Maren  
CS Deutsches Institut fur Ernahrungsforschung (DIFE)-Potsdam, Bergholz-Rehbrücke, D-14558, Germany  
SO Analytical Biochemistry (2000), 278(2), 156-164  
CODEN: ANBCA2; ISSN: 0003-2697  
PB Academic Press  
DT Journal  
LA English  
AB We present the anal. of the stable carbon isotope compns. of 14 individual N-pivaloyl-iso-Pr (NPP) amino acid esters by gas chromatog.-combustion isotope ratio mass spectrometry (GC-C-IRMS). The mean reproducibility of derivatization procedure and GC-C-IRMS anal. was 0.45.permill. (range, 0.12-0.68), whereas the mean anal. error was 0.26.permill. .delta.13C (range, 0.13-0.42). Furthermore, the .delta.13C values of N-pivaloyl-iso-Pr and N-acetyl-Pr (NAP) amino acid esters were compared. Due to a reproducible isotopic fractionation introduced by the derivatization process an empirical correction factor for each individual amino acid was derived sep. for both derivs. (NPP, -1.13 to -2.52 (lysine,

+2.09).permill. .delta.13C; NAP, -2.36 to -3.97 (lysine, +1.91).permill. .delta.13C), and the original .delta.13C value of the underivatized amino acid was calcd. Further, we performed an animal study where rats (n = 5) ingested a mixed meal contg. uniformly 13C-labeled casein (indispensable amino acids 1.3 to 1.7 at. %). One hour after the meal .delta.13C values of protein-bound amino acids from small intestinal mucosa and liver and of free amino acids from mucosa and plasma were detd. Significant 13C enrichments of indispensable amino acids of the free pools of mucosa and plasma (range, 0.0518 to 0.1700 at. % excess) and in mucosa and liver proteins (range, 0.0021 and 0.0161 at.% excess) were obsd. The feasibility of various derivs. for the measurement of carbon isotopic compn. is discussed. (c) 2000 Academic Press.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
TI Processes for producing .beta.-halogeno-.alpha.-amino-carboxylic acids and S-phenylcysteine derivatives and intermediates thereof  
AN 1999:460386 CAPLUS  
DN 131:88201  
TI Processes for producing .beta.-halogeno-.alpha.-amino-carboxylic acids and S-phenylcysteine derivatives and intermediates thereof  
IN Yamashita, Koki; Inoue, Kenji; Kinoshita, Koichi; Ueda, Yasuyoshi; Murao, Hiroshi  
PA Kaneka Corporation, Japan  
SO PCT Int. Appl., 46 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933785	A1	19990708	WO 1998-JP5983	19981228
W: CN, IN, JP, KR, SG, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
			JP 1997-367814 A	19971227
			JP 1998-186314 A	19980701
			JP 1998-264397 A	19980918
EP 1046634	A1	20001025	EP 1998-961624	19981228
EP 1046634	B1	20030910		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
			JP 1997-367814 A	19971227
			JP 1998-186314 A	19980701
			JP 1998-264397 A	19980918
JP 2000186069	A2	20000704	WO 1998-JP5983 W	19981228
			JP 1999-13388	19990121
			JP 1998-186314 A	19980701
			JP 1998-264397 A	19980918
US 6372941	B1	20020416	US 1999-582461	19990816
			JP 1997-367814 A	19971227
			JP 1998-186314 A	19980701
			JP 1998-264397 A	19980918
			WO 1998-JP5983 W	19981228
WO 2000043360	A1	20000727	WO 2000-JP274	20000121
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1067119 A1 20010110 JP 1999-13388 A 19990121  
EP 2000-900854 20000121  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, FI

US 6320072 B1 20011120 JP 1999-13388 A 19990121  
WO 2000-JP274 W 20000121  
US 2000-646702 20001214  
JP 1999-13388 A 19990121  
WO 2000-JP274 W 20000121  
US 2002082450 A1 20020627 US 2001-26732 20011227  
JP 1997-367814 A 19971227  
JP 1998-186314 A 19980701  
JP 1998-264397 A 19980918  
WO 1998-JP5983 W 19981228  
US 1999-582461 A319990816  
US 2002103399 A1 20020801 US 2001-26726 20011227  
JP 1997-367814 A 19971227  
JP 1998-186314 A 19980701  
JP 1998-264397 A 19980918  
WO 1998-JP5983 W 19981228  
US 1999-582461 A319990816

OS CASREACT 131:88201; MARPAT 131:88201

AB Disclosed are an industrially advantageous process for producing .beta.-halogeno-.alpha.-aminocarboxylic acids; and a process for producing optically active N-protected-S-phenylcysteine of formula  $R_1RNCH(CH_2SPh)CO_2H$  ( $R_1$  = amino-protective group;  $R$  = H or R and  $R_1$  together represent an amino-protective group) having a high optical purity and its intermediates with the use of the former process. The process for producing .beta.-halogeno-.alpha.-aminocarboxylic acids or salts thereof comprises treating with a halogenating agent a .beta.-hydroxy-.alpha.-aminocarboxylic acid (wherein the basicity of the amino group at the .alpha.-position is not shielded by the presence of the substituent of the amino group) or a salt thereof with an acid to thereby halogenate the hydroxyl group. The process for producing optically active N-protected-S-phenylcysteine represented by general formula (3) or its salt comprises subjecting optically active serine or its salt to the above-mentioned prodn. process and then treating the product with an amino-protective agent followed by a reaction with thiophenol under basic conditions. These three steps convert optically active serine which is readily available in an industrial scale, into optically active .beta.-chloroaniline and then into N-protected-S-phenylcysteine by reaction of the N-protected-.beta.-chloroaniline with thiophenol without substantially lowering optical purity of the starting material. N-protected-S-phenylcysteine is useful as an intermediate for drugs, in particular anti-AIDS drugs. Thus, 0.4 g L-serine hydrochloride and 0.029 g Et3N were suspended in 4 mL 1,2-dimethoxyethane under N, followed by adding dropwise 0.67 g SOCl2. The resulting mixt. was stirred at 60.degree. for 2 h, treated with 8 mL H2O at 15.degree. and stirred at room temp. for 30 min, treated with 1.6 g K2CO3 to make pH 10, treated dropwise with 0.956 g benzyl chloroformate, stirred at room temp. overnight, ice-cooled, and acidified with 50% H2SO4 to give 42% N-benzyloxycarbonyl-.beta.-chloro-L-alanine (I). To a soln. of 0.108 g I in 0.5 mL H2O was added 0.097 g Na2CO3, followed by adding dropwise 0.054 g thiophenol, and the resulting mixt. was stirred at 60.degree. for 2 h to give, after silica gel chromatog., 81% N-benzyloxycarbonyl-S-phenyl-L-cysteine of 98% e.e.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

TI Molecular analytical release tags and their use in chemical analysis

AN 1997:527647 CAPLUS

DN 127:187872  
 TI Molecular analytical release tags and their use in chemical analysis  
 IN Giese, Roger W.; Abdel-Baky, Samy; Allam, Kariman  
 PA Northeastern University, USA  
 SO U.S., 38 pp., Cont.-in-part of U.S. Ser. No. 45.089.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5650270	A	19970722	US 1990-496251	19900320
				US 1982-344394	19820201
				US 1987-45089	19870504
	US 4709016	A	19871124	US 1982-344394	19820201

PATENT FAMILY INFORMATION:

FAN 1984:20051

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 85554	A1	19830810	EP 1983-300456	19830128
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE			US 1982-344394	19820201
	US 4709016	A	19871124	US 1982-344394	19820201
	DK 8300364	A	19830802	DK 1983-364	19830131
				US 1982-344394	19820201
	ES 519424	A1	19840801	ES 1983-519424	19830131
				US 1982-344394	19820201
	CA 1246058	A1	19881206	CA 1983-420574	19830131
				US 1982-344394	19820201
	JP 58146540	A2	19830901	JP 1983-15359	19830201
				US 1982-344394	19820201
	US 4650750	A	19870317	US 1984-591262	19840319
				US 1982-344394	19820201

FAN 1995:229457

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5360819	A	19941101	US 1985-710318	19850311
				US 1982-344394	19820201
	US 4709016	A	19871124	US 1982-344394	19820201
	DK 8300364	A	19830802	DK 1983-364	19830131
				US 1982-344394	19820201
	ES 519424	A1	19840801	ES 1983-519424	19830131
				US 1982-344394	19820201
	CA 1246058	A1	19881206	CA 1983-420574	19830131
				US 1982-344394	19820201
	JP 58146540	A2	19830901	JP 1983-15359	19830201
				US 1982-344394	19820201
	US 4650750	A	19870317	US 1984-591262	19840319
				US 1982-344394	19820201
	US 5516931	A	19960514	US 1993-53608	19930422
				US 1982-344394	19820201
				US 1985-710318	19850311
	US 5602273	A	19970211	US 1996-598468	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311
				US 1993-53608	19930422
	US 5604104	A	19970218	US 1996-598691	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311
				US 1993-53608	19930422
	US 5610020	A	19970311	US 1996-598439	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311

FAN	1996:350610			US 1993-53608	19930422
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5516931	A	19960514	US 1993-53608	19930422
				US 1982-344394	19820201
				US 1985-710318	19850311
	US 4709016	A	19871124	US 1982-344394	19820201
	US 5360819	A	19941101	US 1985-710318	19850311
				US 1982-344394	19820201
	US 5602273	A	19970211	US 1996-598468	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311
				US 1993-53608	19930422
	US 5604104	A	19970218	US 1996-598691	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311
				US 1993-53608	19930422
	US 5610020	A	19970311	US 1996-598439	19960208
				US 1982-344394	19820201
				US 1985-710318	19850311
				US 1993-53608	19930422
OS	MARPAT 127:187872				
AB	<p>Anal. reagents designated "release tags" are disclosed for labeling mol. species with a highly detectable signal group which can be released in the form of a volatile compd. at a desired point in an anal. procedure. In one embodiment, the release tags have the formula (SgCO)xL(Rx)r wherein each Sg is a signal group bearing .gtoreq.1 electroneg. substituents, L is any of a wide variety of groups which, when attached to a carbonyl group, form a readily cleaved linkage, each COL moiety is a release group which, upon scission, releases signal group Sg in the form of a volatile compd., and each Rx is a reactivity group for attaching the release tag compd. to a mol. species to be labeled. In a second embodiment, the release tags have the formula SgReRx wherein Sg and Rx are defined as above and Re is a release group which is an olefin, .alpha.-hydroxy ketone, or vicinal diol. Conjugates of the release tag compds. with, e.g., proteins, DNA, lipids, carbohydrates, drugs, cells, viruses, pesticides, etc. and assay methods employing them are also disclosed.</p>				
L24	ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN				
TI	Migration of the peptide residue in serine peptides				
AN	1955:24250 CAPLUS				
DN	49:24250				
OREF	49:4741d-h				
TI	Migration of the peptide residue in serine peptides				
AU	Botvinik, M. M.; Avaeva, S. M.; Mistryukov, E. A.				
CS	Moscow State Univ.				
SO	Zhurnal Obshchei Khimii (1954), 24, 2084-91				
	CODEN: ZOKHA4; ISSN: 0044-460X				
DT	Journal				
LA	Unavailable				
AB	<p>cf. C.A. 48, 13628i; Elliott, C.A. 46, 5626g. Treatment of serine peptides contg. other amino-acid groups with SOCl<sub>2</sub> or HCl in alc. or dioxane soln. gave the .beta.-chloro derivs. of alanine peptides which in aq. medium gave the initial compds. Under action of concd. HCl there appears to take place a migration of the peptide union from N to O, since the N-peptides of serine are hydrolyzed more rapidly than O-peptides. Treatment with H<sub>2</sub>SO<sub>4</sub> gave 2 reactions: migration of the peptide link from N to O and dehydration of the peptides. Heating 0.5 g. N-(benzoylphenylalanyl)-serine iso-Pr ester 3 min. with 5 ml. SOCl<sub>2</sub> gave on diln. with Et<sub>2</sub>O N-(benzoylphenylalanyl)-.beta.-chloroalanine iso-Pr ester, m. 157.degree.; the same product formed if SOCl<sub>2</sub> was replaced by dry HCl in dry dioxane. Heating the product 2 hrs. in aq. dioxane soln.</p>				

gave the starting material, m. 168.degree.. N-Benzoylphenylalanylserine methylamide kept 1 hr. with SOCl<sub>2</sub> at 0.degree. gave a product (I), m. 135-7.degree., which on standing evolved SO<sub>2</sub> and gave AgCl ppt. with AgNO<sub>3</sub>; treated with H<sub>2</sub>O it gave the initial amide. I taken up in hot AcOH and dild. with H<sub>2</sub>O gave N-(Benzoylphenylalanyl)-.beta.-chloroalanine methylamide, m. 199.degree.; the same substance formed in reaction with SOCl<sub>2</sub> at 60.degree., PCl<sub>5</sub> in CHCl<sub>3</sub> at room temp., dry EtOH-HCl at 70.degree., or dry dioxane-HCl at room temp. The rate of hydrolysis of N- and O-peptides of serine with acetylphenylalanyl, phthalylglycyl, and benzoylphenylalanyl groups was detd. in concd. H<sub>2</sub>SO<sub>4</sub> by periodic detn. of amino N; similarly hydrolysis was followed of N-(benzoylphenylalanyl)serine iso-Pr ester, N-(benzoylphenylalanyl)serine methylamide, and N-(p-toluenesulfoglycyl)serine methylamide in H<sub>2</sub>SO<sub>4</sub> of various concns. and in concd. HCl at 18-26.degree..

L24 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

TI Oxazolines

AN 1950:40777 CAPLUS

DN 44:40777

OREF 44:7836b-i,7837a-b

TI Oxazolines

AU Fry, Edward M.

CS Natl. Inst. of Health, Bethesda, MD

SO Journal of Organic Chemistry (1949), 14, 887-94

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

AB Because the compd. described as 2-phenyl-4-(carboxymethyl)oxazoline (cf. Bergmann, et al., C.A. 19, 1852) was found to be CH<sub>2</sub>ClCH(NHBz)CO<sub>2</sub>Me (I), the reaction of SOCl<sub>2</sub> with .beta.-hydroxyalkylamides is reinvestigated. Treating CH<sub>2</sub>(OH)CH(NHBz)CO<sub>2</sub>Me (II) with a 4- to 8-fold excess of SOCl<sub>2</sub> in the cold gives a complex salt (III), contg. about 2.1 mols. II and 1 mol. SO<sub>2</sub>, sintering at about 57.degree., m. 108-12.degree.. III seems to be stable in the cold, but at room temp. or on warming it loses SO<sub>2</sub> and H<sub>2</sub>O, giving I. The SOCl<sub>2</sub> in III is bound as an intermediate chlorosulfinate, as is shown by the fact that by passing HCl and SO<sub>2</sub> into an ether soln. of 2-phenyl-4-(carboxymethyl)oxazoline (IV) a similar complex salt is formed. Refluxing II with SOCl<sub>2</sub> gives 86% I, m. 114-16.degree.. Heating I in H<sub>2</sub>O gives 79% CH<sub>2</sub>(OBz)CH(NH<sub>2</sub>.HCl)CO<sub>2</sub>Me (V), m. 137-8.degree., which is also formed in 73% yield when III is dissolved in H<sub>2</sub>O. Decompn. of III in Na<sub>2</sub>CO<sub>3</sub> soln. gives 72% IV, b<sub>2</sub> 133-5.degree., f.p. 29.5.degree., n<sub>D</sub><sup>23</sup> 1.5501. Sapon. of IV gives 2-phenyl-4-carboxyoxazoline (VI), m. 159-61.degree.. Hydrolysis of VI in 95% EtOH at 20.degree. gives 96% O-benzoylserine (VII), m. 145-5.5.degree. (decompn.). VII in Na<sub>2</sub>CO<sub>3</sub> rearranges to 91% N-benzoylserine. Passing HCl into VI in dioxane and heating the mixt. 10 min. give 86% .alpha.-benzamido-.beta.-chloropropionic acid (VIII), m. 145-7.degree., which, heated with H<sub>2</sub>O and treated with HCl-C<sub>5</sub>H<sub>5</sub>N, gives 83% VII. Treating VIII or I with 2 N NaOH at 20.degree. gives 72% .alpha.-benzamidoacrylic acid, m. 153-5.degree. (decompn.), which hydrogenated with Adams catalyst gives DL-benzoylalanine, m. 163-5.degree.. VIII with NaHCO<sub>3</sub> 22 hrs. at 40.degree. gives 50% VI. SOCl<sub>2</sub> (2 mols.) and 1 mol. HOCH<sub>2</sub>CH<sub>2</sub>NHCHO at below 18.degree. give a 1:1 addn. compd., which heated under ether, gives 35% HCONHCH<sub>2</sub>CH<sub>2</sub>Cl b<sub>10</sub> 118.5-21.degree., n<sub>D</sub><sup>25</sup> 1.4845. HOCH<sub>2</sub>CH<sub>2</sub>NHBz (IX) b<sub>1</sub> 179-89.degree., m. 61-3.degree.. Treating 2 g. IX 2 hrs. with SOCl<sub>2</sub> at 0.degree. gives 2.3 g. phenyloxazoline-HCl (X), m. 75-6.degree., which on heating changes to BzNHCH<sub>2</sub>CH<sub>2</sub>Cl (XI), m. 101-3.degree.. X (0.2 g.) heated 2 min. in H<sub>2</sub>O forms 0.133 g. H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OBz.HCl (XII), m. 142-5.degree., and 0.025 g. XI, m. 102-3.5.degree.. XI is also obtained in 88% yield on rearrangement of X on a steam bath. Heating XI 10 min. with H<sub>2</sub>O gives 88% XII. Rearrangement of XII with NaOH gives 61% IX. ClCH<sub>2</sub>CH(OH)CH<sub>2</sub>NH<sub>2</sub> m. 100-3.degree.. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHCH<sub>2</sub>CH(OH)CH<sub>2</sub>Cl (XIII) (74% yield) m. 103-6.degree.. XIII (2 g.) with SOCl<sub>2</sub> gives 2.64 g.



ClCH<sub>2</sub>CH(OSOCl)CH<sub>2</sub>NHCOC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>(p) (XIV) which decompd. with H<sub>2</sub>O gives 1.81 g. XIII. XIV in dioxane with XIII gives 30% bis[3-chloro-1-(p-nitrobenzamido)propyl] sulfinat, m. 167-8.degree. (decompn.). XIV heated in a steam bath loses SO<sub>2</sub>, giving 27% impure p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHCH<sub>2</sub>CHClCH<sub>2</sub>Cl and 73% p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>COCH(CH<sub>2</sub>Cl)CH<sub>2</sub>NH<sub>2</sub>.HCl (XV), m. 185-7.degree. (decompn.). XV treated with NaHCO<sub>3</sub> gives 57% XIII. Heating a suspension of XIV in SOCl<sub>2</sub> 5 min. on a steam bath and evapg. the excess SOCl<sub>2</sub> give 95% 2-(p-nitrophenyl)-5-(chloromethyl)oxazoline-HCl (XVI), m. 127-9.degree. [free base (XVII), m. 116-17.degree.]. XVI loses HCl on standing in the air. Heating XV alone or in SOCl<sub>2</sub> gives N-(2,3-dichloropropyl)-p-nitrobenzamide (XVIII), m. 122-3.5.degree.. With NaOMe XVIII is slowly cyclized to XVII. Heating p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHCH<sub>2</sub>CH(OH)CH<sub>2</sub>Cl (XIX) with Et<sub>2</sub>NH 1 hr. in a sealed tube gives 75% 3-Et<sub>2</sub>N analog-HCl (XX), m. 162-3.5.degree.. Treating 0.3 g. XX with SOCl<sub>2</sub> at 20.degree. and evapg. the SOCl<sub>2</sub> give 20% 2-diethylamino-1-aminopropyl p-nitrobenzoate-2HCl (XXI), m. 194-5.degree. (decompn.). Rearrangement of 2-(p-nitrophenyl)-5-(diethylaminomethyl)oxazoline (XXII)-HCl on a steam bath gives 87% N-(3-diethylamino-2-chloropropyl)-p-nitrobenzamide-HCl, m. 112.5-14.5.degree.. The ease of hydrolysis of XXII is shown by the fact that when 0.5 g. is slowly titrated with N HCl it is completely dissolved after addn. of 1 equiv. HCl (pH 7); after addn. of a 2nd equiv. HCl the pH is 1, and immediate evapn. of the soln. in vacuo gives XXI which, treated 10 min. with NaHCO<sub>3</sub> and acidified, gives 76% XIX.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

27.62

91.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.91

-5.86

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 09:11:22 ON 09 OCT 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

SESSION RESUMED IN FILE 'CAPLUS' AT 09:50:49 ON 09 OCT 2003

FILE 'CAPLUS' ENTERED AT 09:50:49 ON 09 OCT 2003

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

27.62

91.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.91

-5.86

=> d his

(FILE 'HOME' ENTERED AT 08:25:06 ON 09 OCT 2003)

FILE 'STNGUIDE' ENTERED AT 08:25:18 ON 09 OCT 2003

FILE 'HOME' ENTERED AT 08:25:59 ON 09 OCT 2003

FILE 'REGISTRY' ENTERED AT 08:26:08 ON 09 OCT 2003  
E METHYLSELENOCYSTEINE/CN

L1 2 E3

FILE 'CAPLUS' ENTERED AT 08:27:04 ON 09 OCT 2003

L2 112 L1  
L3 367971 AMINE  
L4 2 L2 AND L3  
L5 66 RECEMIZ? OR RACEMIS?  
L6 10436 RACEMIZ? OR RACEMIS?  
L7 0 L2 AND L6

FILE 'CAPLUS' ENTERED AT 08:31:56 ON 09 OCT 2003

FILE 'REGISTRY' ENTERED AT 08:32:21 ON 09 OCT 2003  
E CYSTEINE/CN

FILE 'CAPLUS' ENTERED AT 08:32:21 ON 09 OCT 2003  
S E3

L8 FILE 'REGISTRY' ENTERED AT 08:32:32 ON 09 OCT 2003  
2 S E3/CN

L9 FILE 'CAPLUS' ENTERED AT 08:32:32 ON 09 OCT 2003  
33224 S L8  
L10 86 L6 AND L9  
L11 26 L6(L)L9  
L12 62938 BENZALDEHYDE  
L13 0 L11 AND L12  
L14 2 L10 AND L12  
L15 146703 ALDEHYDE  
L16 1 L11 AND L15

FILE 'CAPLUS' ENTERED AT 09:00:00 ON 09 OCT 2003

FILE 'REGISTRY' ENTERED AT 09:00:06 ON 09 OCT 2003  
E SERINE/CN  
L17 2 E3  
E THIONYL CHLORIDE/CN  
L18 1 E3  
E THIONYL BROMIDE/CN  
L19 1 E3

L20 FILE 'CAPLUS' ENTERED AT 09:01:09 ON 09 OCT 2003  
31363 L17  
L21 5368 L18  
L22 194 L19  
L23 5444 L21 OR L22  
L24 6 L20 AND L23

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

29.70

94.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.91

-5.86

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 09:53:49 ON 09 OCT 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPLUS records now contain indexing from 1907 to the present
NEWS	4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS	5	Jul 21	Identification of STN records implemented
NEWS	6	Jul 21	Polymer class term count added to REGISTRY
NEWS	7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS	8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS	11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS	12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS	13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS	14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS	17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	18	SEP 22	DIPPR file reloaded
NEWS	19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	20	SEP 29	DISSABS now available on STN
NEWS EXPRESS			OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:39:32 ON 09 OCT 2003

=> ogoff hold

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 11:39:42 ON 09 OCT 2003